

Book of Abstracts

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How to use this Book

This Book contains all the abstracts of mini-symposium talks, contributed talks and poster presentations submitted to organisers and scheduled before 28 May 1999. The summaries of Mini-Symposia and the abstracts of Plenary Lectures can be found in the Final Programme.

The book consists of three parts. The first part contains the abstracts of mini-symposia talks grouped by mini-symposia; within each mini-symposium the abstracts are ordered in alphabetical order of speakers' surnames. The second part contains the abstracts of all contributed talks and poster presentations ordered alphabetically. The Index of all Speakers can be found at the end of the Book.

Because of space limitations, only the name of the presenting speaker is included in the Index. Details of co-authors are contained in the abstracts.

The updated electronic version of the Book of Abstracts is available (before, during, and after the Congress) on the ICIAM99 web page,

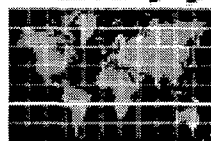
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ICIAM 99

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MSP-001

CONLISK, A Terrence (Ohio State University, USA)

The rotor-tip vortex: Structure and interactions

The helicopter rotor wake is among the most complex structures in aerodynamics. A large amount of computational and experimental work on the rotor wake has been published and much of a qualitative nature is known about the origin of the two main components of the rotor wake: the tip-vortex and the inboard sheet. However, little of a quantitative nature is known concerning the dependence of the very near wake structure (i.e. the circulation, tip-vortex core radius, and initial tip-vortex orientation) on the independent parameters of the flow such as local flow speed, rotor blade geometry and angle of attack. Here we discuss the main features of the origin of the tip-vortex and interactions which can occur with the surrounding solid surfaces such as the rotor blades and the helicopter airframe. The problem is approached from both an experimental and computational perspective. Of particular interest is the case where the vortex directly impacts a rotor blade or fuselage, in which a portion of the vortex core can be destroyed locally. We call this a vortex-surface collision and the behavior of the pressure and swirl velocity within the vortex are described in several examples.

KOMERATH, Narayanan M (School of Aerospace Engineering, Georgia Institute of Technology, Atlanta, USA)

Measurement of vortices generated by rotary wings

Various phenomena observed in rotary-wing vortices, and the issues arising in capturing them, are presented. The vortex system generated by a rotating wing contains a wide range of spatial and temporal scales. Constraints on the dynamic range of analyses and measurements have led to diverse interpretations and approaches. Observations are presented on blade tip flows, wake structure, and vortex-surface interactions. Comparison with computations confirms the experimental evidence that most of these phenomena can be explained using deterministic models.

PAGE, Michael A (Monash University, Australia)

Boundary-layer analysis for rapidly rotating flows

The perturbed motion in a rapidly-rotating and axially-confined fluid shows some novel features that are accessible to a boundary-layer analysis closely related to, and instructed by, the well-known approach for two-dimensional non-rotating flows at high Reynolds numbers. Indeed, the confining effect of the simple additional term in the boundary-layer equations can make the analysis more tractable than for the corresponding non-rotating flow and provides an elegant mechanism for the study of separating flows. This talk reviews some of the progress on the analysis of these flows which has resulted from following the trail of development of modern high-Reynolds-number flow theory.

SMITH, Frank T (University College London, UK)

Rotary blade-wake flows

The main research developments of interest here are in multi-blade motions and their interactions for two- and three-dimensional flows within rotary boundary layers. There are many novel features to be described, in blade-wake flows, in particular for nearly aligned configurations of thin blades (airfoils). All of them require a combination of mathematical theory and accurate computation.

1. Multiple interactions between each viscous blade- and wake-flow;
2. Inner-outer viscous-inviscid interaction at remarkably small incidence;
3. Double viscous layer interactions;
4. Pressure-displacement interactions covering entire blades;
5. Long-scale separations;
6. Short-scale interactions at incidence;
7. Unsteadiness, and transitions in the wakes.

The applications are to helicopters, rotorcraft, fans, turbine flows, domestic and garden appliances, nature, industrial mixers. This is a joint work with S N Timoshin and R G A Bowles (all UCL).

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MSP-002

BORGAS, Michael (CSIRO Atmospheric Research, Australia)

Lagrangian stochastic modelling of dispersion - from theory to practice

Over the last fifteen years the Lagrangian approach to turbulent dispersion has evolved from a rather esoteric research topic to a powerful practical tool for regional modelling studies of atmospheric pollution (so-called Lagrangian particle models). This change has come about due to both advances in the theory and to rapid increases in available computing power. In this paper we give an overview of these developments in the theory and of their practical implementation.

CHATWIN, Philip C (Applied Mathematics, University of Sheffield, UK)

Simple concepts underlying the structure of probabilistic models for concentration and dosage

One motivation for this mini-symposium is the startling increase in the quality of data on the concentration of dispersing pollutants, especially from experiments in the atmosphere and in wind tunnels, that has occurred recently. This has emphasized that quantitative models of concentration and dosage must be probabilistic. It follows that, ultimately, the same must be true for practical models, e.g. for assessing industrial accidents. The talk will emphasize data and discuss the exact equations governing the probability density functions for concentration and dosage, and basic physical arguments that have been used in constructing simple models. This is a joint work with Nils Mole, University of Sheffield, UK.

NIELSEN, Morten (Risoe National Laboratory, Denmark)

Prediction of concentration fluctuations by combination of a Plume-Meander model and an empirical stochastic model for in-plume fluctuations

Concentration time series downstream of a continuous gas source in the atmosphere should be considered a stochastic process. So should the time-averaged concentration field since the time scales of the dispersion process may be as long as the release duration. We reduce the variability by separating the problem into 1) a model for the meandering plume dimensions and centre-line position and 2) a semi-empirical model for the random in-plume fluctuations. The stochastic sub-model applies input from atmospheric boundary layer parameters, source configuration, plume dimensions, and receptor position. This is a joint work with Hans E Joergensen and Soeren Ott.

SULLIVAN, Paul J (Applied Mathematics, University of Western Ontario, Canada)

The PDF of scalar concentration

A case is made for the probability density function to be a mixture of two PDFs and physical arguments and some experimental evidence is adduced in support of this contention. Constraints on the possible forms of the PDFs in the mixture are explored. A plausible application of extreme value analysis in statistics along with an interpretation of the widely observed, ostensible quadratic dependence of kurtosis on skewness suggest the beta PDF for both components of the mixture as one possibility (not the only one). The double beta is shown to well represent some wind tunnel plume data. This is a joint work with Tom Schopflicher, University of Western Ontario.

YEE, Eugene (DRE Suffield, DND, Canada)

Probability theory as logic for representation of uncertainty in turbulent diffusion problems

The conceptual basis underlying the mathematical description of turbulent diffusion by probability distributions is examined critically. It is recognized that the basic role of probabilities in turbulent diffusion is to provide a means for describing a state of (incomplete) human knowledge about the phenomenon. The various methods (e.g., fluctuating plume model, maximum entropy principle) that have been used to assign probability distributions to represent this state of knowledge will be discussed.

MILLS, Graham (CSIRO, Australia)

Network models for workforce allocation

We consider non cyclic rosters which include a limited number of work patterns followed by off stretch patterns. Millar and Kiragu (1998) developed a network model for allocation of the workforce to cover demand. Our method generates column with similar work patterns and off stretches. A set covering model is used to optimise the allocation of the workforce. We compare the results for the network and set covering approaches. This is a joint work with Guy Eitzen, CSIRO and University of South Australia.

PANTON, David M (University of South Australia, Australia)

Column generation models for optimal workforce allocation with multiple breaks

We consider the optimal allocation of a workforce to shifts which include multiple breaks. Recent work by Aykin (1998) presents an implicit branch and cut algorithm with rounding heuristics. Our model uses set covering incorporating column generation techniques. Two approaches are discussed. The first generates optimal non-break solutions for which all break variations are generated and added to the model. This approach is repeated with appropriate costing of non-break columns until an "optimal" solution is found. The second uses a classical column generation approach starting with a restricted set of break columns. Results are discussed and compared for both models. This is a joint work with Professor David Ryan, Engineering Science, University of Auckland, New Zealand.

RYAN, David M (Department of Engineering Science, University of Auckland, New Zealand)

Optimised cell batching for an aluminium smelter

Aluminium is produced by the electrolytic reduction of alumina in cells which are arranged in long lines. The purity of aluminium varies from cell to cell. High purity aluminium commands a premium price on the metals market. Molten metal is tapped from cells into crucibles which are used to transport the metal to casting furnaces. Each crucible taps metal from three cells that are located within some specified limit of spread. This paper describes the development of a set partitioning optimisation model to batch cells for tapping so that the total premium value of metal is maximised. Numerical results show that significant improvements of between 10 and 20 percent can be achieved.

SIER, David (CSIRO, Mathematical and Information Sciences, Australia)

Rostering ambulance officers: Network based algorithms

We describe a system developed to roster the officers for a state ambulance service. The rosters are made up of alternating patterns of work shifts and off periods that can be generated by the rostering officer. The objective is to match the demand for a certain number of officers on duty for each shift type on each day over a year long planning horizon.

A number of solution methods, MILP, shortest path and heuristic, are considered. The method finally adopted is discussed together with the system interface used for the delivered product.

This is a joint work with Ernst, Hourigan, Krishnamoorthy and Nott.

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MSP-004

ARNOLD, Anton (TU-Berlin, Berlin, Germany)

The stationary boundary value problem for the Wigner equation

The pseudo-differential Wigner equation is a kinetic formulation of quantum mechanics which is essentially equivalent to the Schrödinger equation. Recently, Wigner models became an important tool for simulating the electron transport in sub-micron semiconductor devices. In this talk we shall discuss the well-posedness of the stationary boundary value problem for the linear Wigner equation on a slab of the phase space with inflow boundary conditions (BCs). In contrast to the classical Liouville equation, where closed trajectories may appear inside the domain, the quantum problem is uniquely solvable. In the analysis of this "forward-backward problem" we construct the propagator that maps left BCs onto right BCs (and v.v.) to prove the solvability.

DOLBEAULT, Jean (Univ. Paris IX, CEREMADE, Paris, France)

Asymptotic dispersion profile for kinetic equations and related models

Rescalings have been used for a long time in the study of large time asymptotics of partial differential equations. Basically, they allow to build self-similar solutions which are giving the asymptotic behaviour of the solutions to the Cauchy problem. The main drawback is that self-similar solutions correspond to singular initial data. Time-dependent rescalings avoid this difficulty and are especially convenient to work in relative entropy frameworks.

POUPAUD, Frédéric (Laboratoire J A Dieudonne, Universite de Nice, France)

Semiclassical limits in crystals

We present rigorous mathematical results concerning the semi-classical limits of Schrödinger equations in semiconductors. The two small parameters in the equations are related to the Planck constant and to the characteristic length of the period of the semiconductor lattice. The asymptotics is performed via the Wigner formalism. In the limit the observables are given by moments of a distribution function which solves the Boltzmann transport equation of semi-conductors. As a consequence we prove the occurrence of Brillouin oscillations. Application of the theory to super-lattices modelling will also be given.

SOLER, Juan (Granada University, Spain)

On Wigner/Schrödinger-type equations with dissipation and scattering effects for semiconductor devices: Stability and asymptotic behaviour

The evolution of an electron in a cristal, including scattering effects, is analyzed in both Schrödinger and Wigner representations, obtaining new terms in the corresponding systems. Some special cases are derived as a new kinetic Wigner equation for a single electron moving in an electric field and undergoing phonon scattering in the limit of weak electron-phonon coupling where we use the Fröhlich hamiltonian and particularize the new equation for an electron moving in a simple periodic potential under constant electric field. Generalizations considering the electron-electron interaction in the Hartree approximation are also given.

TOSCANI, Giuseppe (Dipartimento di Matematica, Universita' di Pavia, Italy)

Logarithmic Sobolev inequalities for kinetic semiconductor equations

In this paper we analyze the convergence rate of solutions of certain drift-diffusion-Poisson systems to their unique steady state. These bi-polar equations model the transport of two populations of charged particles and have applications for semiconductor devices and plasmas.

When prescribing a confinement potential for the particles we prove exponential convergence to the equilibrium. Without confinement the solution decays with an algebraic rate towards a self-similar state. The analysis is based on a relative entropy type functional and it uses logarithmic Sobolev inequalities.

EGGER, Joseph (Meteorologisches Institut, Universitaet Muenchen, Germany)

Nonhydrostatic mountain effects

Gravity waves as induced by mountains may be strongly nonhydrostatic. The related linear theory is reviewed with particular emphasis on nonhydrostatic ray paths and on conditions for wave breaking. Gravity waves affect the atmospheric large scale flow and climate via their momentum transports. In particular, mean flow momentum is removed nonhydrostatically in regions of wave breaking. Observational evidence for this process is reviewed and related parameterization schemes are discussed.

GREVE, Ralf (Institut für Mechanik III, Technische Universität Darmstadt, Germany)

Ice-sheet modelling beyond the shallow-ice approximation

The model equations which are typically applied in dynamic/thermodynamic simulations of large ice sheets like Greenland and Antarctica make use of the *shallow-ice approximation* (SIA). In this limit, the ice motion is governed by hydrostatic pressure and bed-parallel shear stress, the effect of normal stress deviators is neglected. The large-scale behaviour of ice sheets can be very well described with the SIA; however, it breaks down in the vicinity of ice domes and close to the margin. Especially the former restriction is of practical relevance, because deep ice cores are often drilled at domes in order to obtain very old ice. Therefore, simulations of the Greenland ice sheet are discussed, where the ice sheet as a whole is described by the SIA, and for a 160-km window around Summit (the highest point of Greenland) a locally refined grid is applied, on which the normal stress deviators are taken into account in addition.

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 MSP-005

SANDER, Johannes (Climate and Environmental Physics, Physics Institute, University Bern, Switzerland)

Production of deep water in the open ocean and lakes: Results from a non-hydrostatic model

Renewal of deep water plays a significant role in many prominent geophysical processes reaching from global scale of the thermohaline circulation to ventilation of lakes. Production of deep water takes place in very limited areas and only during short periods of time. Then, the vertical acceleration of parcels of water becomes large and the hydrostatic assumption is violated. For different types of flow scaling arguments are given for the hydrostatic assumption to hold. Numerical calculations with fully non-hydrostatic equations are presented and results are compared with adjustment algorithms under the hydrostatic assumption. Calculations have been performed and validated for heat and wind driven circulation of deep reaching mixing in the ocean and lakes.

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BERGER, Mitchell A (Mathematics, University College London, UK)

Quantitative measures of topological complexity for fluids and magnetic fields

This talk will review observations of topological structure in flows and magnetic fields, and discuss its origin and effects. The internal structure of a magnetic field or flow field can be quantified using helicity integrals and crossing number integrals. Helicity measures net twist and linking. The build up of magnetic helicity in the solar corona can lead to dramatic releases of energy and plasma into space. Crossing numbers provide a measure of topological complexity for knots and links. These numbers can also be used to describe continuous vector fields. They provide estimates for the energy of a complex field structure.

GAMBAUDO, Jean-Marc (UMPA, ENS-Lyon, France)

Asymptotic invariants for volume preserving flows

For a volume preserving flow in a 3-dimensional space, we know from the Poincaré recurrence Theorem that almost all trajectories are recurrent. When closing such trajectories (using a shortest geodesic for instance), we get a knot (one trajectory) or a link (more than one trajectory) to which we can associate the whole panoply of invariants we have at our disposal (linking number, Alexander polynomial, signature, etc.). The subject of this talk is to discuss how these invariants behave in average when time increases and to relate the knowledge of these asymptotic invariants to the dynamical properties of the flow and their applications to fluid dynamics.

GHRIST, Robert W (Georgia Institute of Technology, USA)

Knotted flowlines in steady 3-D Euler flows

We consider the topological properties of flowlines in steady solutions to the Euler equations. By employing topological techniques emanating from the study of contact structures, we prove topological theorems about the solutions: i.e., the theorems hold regardless of the metric underlying the flow.

For example, we show that under certain regularity conditions, steady Euler flows on the three-sphere always possess periodic orbits which are unknotted. Likewise, we can construct examples of smooth, steady Euler flows which exhibit all possible knotting of orbits simultaneously.

HOLMES, Philip J (Princeton University, USA)

Why knot? Some links among topology, dynamics, and bifurcations

This brief introductory talk will sketch some history and set the scene for the lectures to follow in the minisymposium. In particular I will describe some applications of knot invariants to the study of global bifurcations of three-dimensional flows and their associated two-dimensional Poincaré mappings.

BOSSAVIT, Alain (Électricité de France, Clamart, France)

The curl-curl operator, from a geometrical viewpoint

The use of vector fields in electromagnetism is open to criticism. As we intend to argue, differential forms should displace them, on the following grounds. Th is formalism (1) neatly separates equations into two groups: the fully covariant Ampère and Faraday's laws on the one hand, and the metric-dependent constitutive laws on the other hand; thus refraining to introduce a metric before it's really needed helps clarify a lot of issues (symmetry of Maxwell equations, local force computations ...) (2) has a straightforward discretization, thanks to Whitney forms (which are to differential forms what ordinary finite elements are to functions), with here also a welcome clarification of the concept of "mixed" elements. As a demonstration of its power, we shall address the notorious "curl-curl" equation in magnetostatics, $\text{rot}(\mu^{-1}\text{rota}) = j$. Both practical problems of non-uniqueness of a (should one "gauge" a or not?) and non-existence (when j is not properly discretized) find neat solutions in terms of Whitney forms.

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FERNANDES, Paolo (Istituto per la Matematica Applicata del Consiglio Nazionale delle Ricerche, Italy)

Dealing with realistic assumptions in electromagnetics

When developing a computational model, well-posedness of the continuous model we are discretizing should be always proved. In electromagnetic applications, however, the mathematical tools available in the literature do not permit to work out this task, even for models that in engineering practice are regarded as fairly simple. In fact, the assumptions under which some basic results are obtained exclude important features that are very common in a realistic electromagnetic model.

In order to deal with realistic assumptions in electromagnetics, we generalise classical orthogonal decompositions of square integrable vector fields and some related results.

This is joint work with Gianni Gilardi, Dipartimento di Matematica dell Università di Pavia, Italy.

PERUGIA, Ilaria (Dipartimento di Matematica, Università di Pavia - Italy)

An adaptive field-based method for magnetostatic problems

A mixed field-based formulation for magnetostatics will be compared with potential-based approaches. The formulation minimises the residual of the constitutive equation, and exactly imposes Maxwell's equations with Lagrange multipliers. The most natural vector interpolators for both the magnetic and the magnetic induction fields are used to overcome the unsatisfactory behaviour of potential-based formulations in the neighbourhood of sharp discontinuities in material properties. The proposed approach allows the definition of a very natural error estimator which is used to guide the adaptive mesh refinement procedure. Furthermore, the conditions under which the formulation can be decomposed in two separate sets of equations will be discussed. This is a joint work with P Alotto, Department of Electrical Engineering, University of Genoa.

TROWBRIDGE, Bill (Vector Fields Ltd)

A review of potential formulations for Eddy current problems with particular attention to the Lorentz gauge

Low frequency electromagnetic field problems can be solved utilising the finite element method with great efficiency by representing the field quantities through a suitable combination of vector and scalar potentials. However, the efficiency of such solutions depends upon, and is significantly affected by, the choice of partially arbitrary but mathematically necessary conditions which are not directly related to the underlying physical laws. (See: C F Bryant, C R Emson, C W Trowbridge and P Fernandes "Lorentz gauge formulations for eddy current problems involving piecewise homogeneous conductors", Presented at the COMPUMAG '97 Conference, To be published in IEEE.) This paper will review the standard potential formulations for Eddy Current Problems, and will explore the scope of these partially arbitrary conditions and their significant impact upon the efficiency of solution, with particular attention to the Lorentz gauge. This is a joint work with C F Bryant and C R I Emson, Vector Fields Ltd, Oxford, UK and P Fernandes, Istituto per la Matematica Applicata, Genova, Italy.

BERTRAND, Olivier (IRISA/INRIA-Rennes, France)

Counting the Eigenvalues which lie in a region of the complex plane.

We present different methods to count the eigenvalues surrounded by a piecewise C^∞ Jordan curve in the complex plane. They are based on the computation of the Cauchy integral formula along this closed curve. This leads to follow a determination of the complex logarithm by a numerical quadrature. We present several stepsize controls based on: - an expansion of the logarithm. - the trapezoidal rule with constant or variable stepsize. - quadrature from interpolating polynomials.

Numerical experiments show for different tests the advantage and disadvantage of each method. A parallel code has been developed and applied to the study of the stability of flows in hydrodynamics. This is a joint work with B Philippe (IRISA-Rennes).

FRAYSSÉ, Valérie (CERFACS, France)

Pseudospectra at CERFACS

In this presentation, we survey the most recent works about pseudospectra realized in the Qualitative Computing Group at CERFACS. The first part is dedicated to pseudospectra of matrices and their relationships with backward error analysis. Different classes of perturbations are considered, in particular normwise perturbations and homotopic perturbations. We also show that this latter class of perturbations is an efficient tool for revealing the most influent Jordan structure in the neighborhood of a matrix.

The second part is devoted to pseudospectra of operators. The notion of convergence of a family of operators (T_n) which ensures the convergence of the pseudospectra $\sigma_\varepsilon(T_n)$ is addressed for bounded operators in a Banach space. The sensitivity of pseudospectra to the discretization scheme is illustrated on specific differential operators such as the convection-diffusion operator.

GRAMMONT, Laurence (UMR CNRS, Université de Saint-Étienne, France)

Pseudospectrum: The principle of the thing

The ε -spectrum has been introduced in two different ways : with the resolvent in order to generalize the notion of an eigenvalue and as a perturbation tool, $\{z \in \mathbb{C} : \exists E \in \mathbb{C}^{n \times n}, \|E\|_2 \leq \varepsilon \text{ and } z \in \text{sp}(A+E)\}$. We first propose other ways to define it and set assumptions under which these definitions are equivalent. This leads us to think that the choice of the spectral norm in the definition of the ε -spectrum is the most interesting one, both theoretically and computationally.

Second, we investigate the nature of this mathematical object: we study the influence on it of the nonnormality and we state some results about ε -spectrum of partitionned matrices. This is joint work with S Chamier and A Largillier.

SADKANE, Miloud (Department of Mathematics, Université de Bretagne Occidentale, Brest, France)

Computation of pseudospectra by means of an harmonic l^1 approximation

The pseudospectrum concept has gained an important place in numerical matrix analysis. However, in spite of a tremendous development both in theoretical and algorithmic areas, the practical computation of pseudospectra is still very expensive and stay a challenging task.

Considering the subharmonic properties of the resolvent norm, we propose its approximation by an harmonic function on domains with holes excluding the singularities i.e. the eigenvalues. The harmonic function is computed by means of a finite element discretization, imposing Dirichlet type boundary conditions set to the exact values of the resolvent norm. The low cost connected with the computation of the harmonic function allows to consider extremely fine grids of the complex plane.

Our aim is to demonstrate the validity of this approach and enlight the range of problems where this approximation leads to valuable results.

TREFETHEN, Lloyd N (Oxford University, UK)

Applications of pseudospectra in physics

The best known physical applications of pseudospectra are in the field of hydrodynamic stability, but other physical applications are getting attention recently. Several examples will be discussed including lasers, non-hermitian quantum mechanics, and chemical kinetics.

KLAR, Axel (FU Berlin, Germany)

Numerical low Mach number limit for kinetic equations

In this talk numerical methods for kinetic equations working uniformly in the low Mach number limit are discussed. Numerical schemes for a discrete velocity model based on a Lattice-Boltzmann approximation and for the Boltzmann equation are considered in the incompressible Navier-Stokes limit. The schemes are induced by the asymptotic analysis of the Navier-Stokes limit for the Boltzmann equation. They work uniformly for all ranges of mean free paths. In the limit the schemes reduce to the Chorin projection method for the incompressible Navier-Stokes equations. Numerical results for different physical situations are shown and the uniform convergence of the scheme is established numerically. Literature: A.Klar, An asymptotic induced numerical method for kinetic equations in the low Mach number limit, to appear in SIAM J. Num. Anal.; A.Klar, Relaxation scheme for a Lattice-Boltzmann type discrete velocity model and numerical Navier-Stokes limit, to appear in J.Comp.Phys.

MAJORANA, Armando (Dipartimento di Matematica, Universita' di Catania, Italy)

Spherical-harmonic type expansion for the Boltzmann equation in semiconductor devices: Numerical results

The Boltzmann equation for an electron gas in a semiconductor is considered. The electron energy is assumed to have a very general form, so that, for instance, parabolic or non parabolic band approximations can be treated. A technique, which recalls the classical moment method due to Grad, to deduce approximate kinetic models is briefly shown and compared with the *spherical harmonic expansion*. In such deduced models the unknown functions depend on the space-time coordinates and the electron energy. So, they represent transport equations. They have many important features (e.g., an entropy inequality holds), which are equivalent to those of the Boltzmann equation. By using these models a few typical phenomena are studied. The numerical results are shown and compared with those obtained by hydrodynamical or statistical approaches.

MAS-GALLIC, Sylvie (Université Evry-Val-d'Essonne and Ecole Polytechnique CMAP, France)

Diffusion velocity method: Applications to kinetic problems

The diffusion velocity method is a purely lagrangian method based on the application of Fick's law to the flux. It was first introduced in the context of plasma physics. The basic idea was developed by J Fronteau and X Combis for a model Fokker-Planck equation. P Degond and F J Mustieles have adapted it to a general advection-diffusion equation and to a two-dimensional model Fokker-Planck equation. Recently it has been successfully applied to solve approximately problems of viscous incompressible fluid mechanics such as the three-dimensional Navier-Stokes equations. In this contribution, we will present some applications to kinetic models with collisions. This is a joint work with G Lacombe, Université Evry-Val-d'Essonne, France.

RUSSO, Giovanni (Dipartimento di Matematica, Università dell'Aquila, Italy)

Spectral methods for the Boltzmann equation

In this talk we present new spectrally accurate and efficient schemes for the numerical solution of the Boltzmann and the Landau-Fokker-Planck equation, developed in collaboration with L Pareschi. The schemes can be designed to preserve the positivity of the solution and the total mass, whereas momentum and energy are approximated with infinite-order accuracy. Consistency and stability of the methods are also proved. The Fourier coefficients associated to the collision kernel of the equation have a very simple structure and in some cases can be computed explicitly. Numerical examples for homogeneous test problems in two and three dimensions confirm the advantages of the method.

SCHMEISER, Christian (TU Wien, Austria)

Semiconductor device simulation by higher order moment systems

Moment systems with variable order are used as an approach for the numerical solution of semiclassical kinetic models for charge transport in semiconductor devices such as the MOSFET. In particular, an adaptive and locally varying choice of the the order leads to an alternative to domain decomposition approaches, where macroscopic and kinetic models are used in different subdomains. Among other topics, adaptive order strategies, semi-implicit space-time discretizations, and the implementation of boundary conditions will be discussed. Also the results of two-dimensional MOSFET-simulations will be presented.

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MSP-011
MSP-242

BAXENDALE, Peter H (University of Southern California, USA)

Bifurcation theory for stochastic differential equations

In many physical systems which can be modelled by Itô stochastic differential equations, the equilibrium and stability properties of the system change as certain parameters in the system vary. Stationary probability measures may appear or disappear; (almost surely) stable fixed points may become (almost surely) unstable; pairs of trajectories may diverge (almost surely) instead of converging. Very often these phenomena are associated with the change of sign of a relevant Lyapunov exponent. In this talk we shall give some examples and results concerning such systems.

FREIDLIN, Mark (University of Maryland, USA)

Stochastic behaviour of perturbed Hamiltonian systems

I will consider long time behavior of deterministically perturbed Hamiltonian systems. In the case of one degree of freedom, the slow component of such a deterministic dynamical system, in a proper timescale, should be considered as a stochastic process on a graph corresponding to the Hamilton function. In the case of many degrees of freedom the corresponding process should be considered on a complex which is defined by the first integrals of the non-perturbed system. I will discuss both cases, one and many degrees of freedom.

IMKELLER, Peter (Humboldt-Universität zu Berlin, Institut für Mathematik, Berlin, Germany)

Explicit description and global properties of Lyapunov exponents and rotation numbers of systems generated by two-dimensional stochastic differential equations

The Lyapunov exponents of the linearization $\dot{x} = -x + \beta\dot{x} + \sigma \xi_t x$ of a two-dimensional noisy Duffing-van der Pol oscillator are key quantities in the investigation of the stochastic Hopf bifurcation of this system. We derive a simple equation exhibiting them explicitly as functions of the fourth moment of the invariant measure of an associated linear diffusion with drift given by a potential function and additive noise. As a result of this, they can be explicitly expressed in terms of hypergeometric functions. This representation leads to different kinds of complete asymptotic expansions, as well as a rather complete account of global properties of the Lyapunov exponents as functions of β and σ . The approach can be generalized to the class of two dimensional systems for which the noise matrix in the linearization is of triangular type. It covers for example the case of the noisy inverted pendulum. The approach provides explicit descriptions of the rotation numbers of the systems as well.

NAMACHCHIVAYA, N Sri (University of Illinois, Urbana-Champaign, USA)

Stochastic stability and bifurcation

Sample or almost-sure stability of a stationary solution of a random dynamical system is of importance in the context of dynamical systems theory, due to its connection to Lyapunov exponents, and from the point of view of applications, since it guarantees all samples except for a set of measure zero tend to the stationary solution as time goes to infinity. In this paper we construct an asymptotic expansion for the maximal Lyapunov exponent (see M M Doyle and N Sri Namachchivaya, *Almost-Sure Asymptotic Stability of a General Four Dimensional Dynamical System Driven by Real Noise*, J Stat Physics, vol 75(3/4), 525-552 (1994)) and the moment Lyapunov exponents (see N Sri Namachchivaya, H J Van Roessel and M Doyle, *Moment Lyapunov Exponent for Two Coupled Oscillators Driven by Real Noise*, SIAM Jour Appl Math, vol 75(3/4), 525-552 (1994)) for random dynamical systems driven by a small intensity real noise process. The results obtained are applied to gyroscopic mechanical systems which are encountered in many engineering applications (see Vincent Nolan and N. Sri Namachchivaya, *Almost-Sure Stability of Gyroscopic Systems Driven by Real Noise*, J Sound Vibration, to appear). In order to formalize this qualitative change in the stochastic context, two approaches have been pursued so far. They are called *the phenomenological approach* (P-bifurcation) and *the dynamical approach* (D-bifurcation). The moment Lyapunov exponent provides insight into the response of the full nonlinear equations of motion. It provides the parameter value necessary to attain a normalizable density function for the nonlinear response and parameter values at which this density function undergoes qualitative changes. This is joint work with Henry Van Roessel, University of Alberta, Canada.

SOWERS, Richard (University of Illinois, Urbana-Champaign, USA)

Stochastic dynamical systems: Asymptotic and averaging

In this paper we will discuss some asymptotic questions relating to stochastic averaging of physically-motivated stochastically-perturbed nonlinear Hamiltonian systems. We will discuss rates of convergence and the effects of critical points of the Hamiltonian. At these critical points, gluing conditions govern the Fokker-Planck equation for the density of the averaged Markov process. Of particular interest is the behavior of the boundary layer near the critical points of the Hamiltonian. This is joint work with N Sri Namachchivaya.

WEDIG, Walter V (Institut für Technische Mechanik, Universität Karlsruhe, Germany)

Stationary solutions of higher-dimensional Fokker-Planck equations

The paper investigates approximated solutions of multi-dimensional Fokker-Planck equations to obtain stationary probability densities of non-linear dynamical systems driven by random noise excitations. The analytical solutions are compared with corresponding results of Monte-Carlo simulations. Several applications are considered. First, the Duffing-van der Pol oscillator under additive coloured noise is investigated. Stochastic averaging is performed by introducing spherical coordinates with an amplitude, an angle of rotation and one fluctuating angle. Associated stationary densities are calculated by generalized polynomials and Fourier expansions. Extensions of this application are given for the four-dimensional problem of two coupled oscillators under white noise and for the six-dimensional case of two coupled oscillators excited by Ornstein-Uhlenbeck processes. This is joint work with Utz von Wagner.

WIHSTUTZ, Volker (University of North Carolina, Charlotte, USA)

Stability maps for systems with noise induced stability

A system like an inverted pendulum standing on a membrane can be stabilized by randomly vibrating the supporting membrane, provided suitable noise is used. [White noise, d(Wiener), is not suitable, for example, but d(Ornstein-Uhlenbeck) is.] The originally unstable equilibrium becomes stable, if the top Lyapunov exponent is associated with the noise perturbed system becomes negative. Stochastic numerical schemes are discussed to compute λ as function of the damping b and the noise intensity $1/\epsilon$ for such a system; in particular, the border line $\lambda(b, \epsilon) = 0$ is considered.

JONES, Christopher K R T (Brown University, USA)

Viscosity and transport in ocean models

Recent developments in dynamical systems have afforded the application of geometric techniques to strongly time-dependent flows. These techniques can be used to determine the redistribution of fluid around coherent features, such as jets and eddies. (Eddy) viscosity is usually included in generating such models and it plays a significant role in promoting transport, but the primary effect can be to produce transport that is non-chaotic as shown in work of the speaker with Balasuriya and Sandstede. The extent to which the transport of active scalars, such as vorticity, can be deduced from the geometric analysis will be addressed through a discussion of recent results of Haller and Poje.

KING, Gregory P (University of Warwick, UK)

The Taylor-Couette reactor

The flow between rotating cylinders (Taylor-Couette system) is a favourite test bed for theoretical and experimental studies of stability and transition. Because so much is known about the flows occurring in the Taylor-Couette system, we chose it for our investigations of chaotic advection in three-dimensional fluid flows (see P Ashwin and G P King, *Streamline Topology in Eccentric Taylor-Vortex Flow*, J. Fluid Mech. 285 (1995) 215-247 and P Ashwin and G P King, *A study of particle paths in non-axisymmetric Taylor-Couette flows*, J. Fluid Mech. 338 (1997) 341-362). For the same reason, engineers are investigating its use as a novel reaction vessel and as a dynamic filter. Such applications need a better understanding of the transport and mixing behaviour in different flow regimes, thus prompting the recent study of particle paths in Navier-Stokes simulations of wavy Taylor-vortex flow by Murray Rudman of CSIRO (Australia) (see M Rudman, *Mixing and Particle Dispersion in the Wavy Vortex Regime of Taylor-Couette Flow*, AIChE J. 44 (1998) 1015-1026).

In this talk I will review our previous work and describe some recent results we have obtained applying our recently proposed Eulerian diagnostic for Lagrangian chaos (see A N Yannacopoulos, I Mezic, G Rowlands and G P King, *An Eulerian diagnostic for Lagrangian chaos in three dimensional Navier-Stokes flows*, Phys. Rev. E 57 (1998) 482-490) to Rudman's simulations.

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MSP-012

PIRO, Oreste (Mediterranean Institute of Advanced Studies (IMEDEA), CSIC-University of Balearic Islands, Spain)

Chaotic advection in three-dimensional incompressible flows

In this talk we will briefly review the way in which the global aspects of advection by non-turbulent but time-dependent three-dimensional incompressible fluid flows are described by volume-preserving (Liouvillian) three-dimensional maps. An interesting phenomenon appearing in this description is the existence of global diffusion of passive-scalar particles at arbitrarily small values of the nonintegrable perturbation. We study a model of an experimentally realizable flow which display this type of chaotic advection, termed *resonance-induced diffusion* to analyze both qualitatively and quantitatively its impact on mixing efficiency.

On the other hand, generic behavior of Liouvillian maps suggests also the existence transport barriers similar to those displayed by two-dimensional flows. Evidence of these barriers in few model systems will be discussed.

TÉL, Tamás (Institute for Theoretical Physics, Eötvös University, Budapest, Hungary)


Chemical or biological activity in open chaotic flows

We investigate the evolution of particle ensembles in open chaotic hydrodynamical flows. Active processes of the type $A + B \rightarrow 2B$ and $A + B \rightarrow 2C$ are considered in the limit of weak diffusion. As an illustrative advection dynamics we consider a model of the von Kármán vortex street, a time periodic two-dimensional flow of a viscous fluid around a cylinder. We show that a fractal unstable manifold acts as a catalyst for the process, and the products cover fattened-up copies of this manifold. This may account for the observed filamental intensification of activity in environmental flows. The reaction equations valid in the wake are derived either in the form of dissipative maps or differential equations depending on the regime under consideration. They contain terms that are not present in the traditional reaction equations of the same active process: the decay of the products is slower while the productivity is much faster than in homogeneous flows. Both effects appear as a consequence of underlying fractal structures. In the long time limit, the system locks itself in a dynamic equilibrium state synchronized to the flow for both types of reactions.

YANNACOPOULOS, Athanasios N (School of Mathematics and Statistics, University of Birmingham, UK)

Chaotic advection in biofluids

Chaotic advection may have some interesting applications in biological fluid dynamics. Its effects on mixing and transport in some simple models of internal or external slow viscous flows of biological significance will be discussed.

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 MSP-013

CARRILLO, José A (Department of Mathematics, University of Texas at Austin, Texas, USA)

Some results about nonlocal problems with decreasing nonlinearity of exponential type

In this talk I will focus on the existence of classical solution for the nonlocal elliptic equation $-\Delta u = \alpha e^{-u} (\int_{\Omega} e^{-u} dx)^{-p}$ in Ω with homogeneous Dirichlet boundary condition ($u = 0$ on $\partial\Omega$), depending on the values of the parameters $\alpha > 0$ and $p > 0$.

For $p = 1$ this problem appears in statistical mechanics and is called the Poisson-Boltzmann equation. The case $p = 2$ is a model for heat evolution in electrical conduction. We describe the existence of solution of this problem depending on p . In fact, this problem satisfies that: (1) If $p \leq 1$, there exists a unique solution for any $\alpha > 0$. (2) If $1 < p < 2$, there exists at least a solution for any $\alpha > 0$. (3) If $p = 2$, there exists a critical value α_2^* such that there exists at least a solution for any $0 < \alpha \leq \alpha_2^*$ and no solution for $\alpha > \alpha_2^*$. (4) If $p > 2$, there exists a critical value α_p^* such that there exist at least two solutions for any $0 < \alpha < \alpha_p^*$, at least a solution for $\alpha = \alpha_p^*$ and no solution for $\alpha > \alpha_p^*$.

This result can be improved for a convex domain.

CHIPOT, Michel (Universität Zürich, Institut für Mathematik, Zürich, Switzerland)

On the asymptotic behaviour of some nonlocal problems

We would like to consider problems of the type
$$\begin{cases} u_t - a(l(u(\cdot, t)))\Delta u = f & \text{in } \Omega \times (0, T), \\ u(\cdot, t) \in H_0^1(\Omega), & t \in (0, T), \\ u(x, 0) = u_0(x) & \text{in } \Omega \end{cases} \quad \text{where } l \text{ is}$$

for instance a linear continuous functional on $H_0^1(\Omega)$. In particular we will investigate the question of the asymptotic behaviour of u toward the multiple steady states that are associated to these problems.

LACEY, Andrew A (Heriot-Watt University, UK)

Thermal runaway in nonlocal models of Ohmic heating

Equations of the form $u_t = \Delta u + \lambda f(u) / (\int_{\Omega} f(u) dx)^p$ are derived as models for the temperature u in a region Ω through which an electric current is flowing. A comparison principle for cases in which f is a decreasing function allows the use of upper and lower solutions to estimate u . In particular, in one dimension with $p = 2$ and homogeneous Dirichlet boundary conditions: for f decreasing global blow-up occurs if λ is so large that no steady state exists but for smaller λ any steady solution is globally asymptotically stable; if f is positive and bounded away from zero then u is bounded.

SOUPLET, Philippe (Département de Mathématiques, Université de Picardie, France)

Blowup behaviour in nonlocal versus local reaction-diffusion equations

We present some recent results on blowup for parabolic equations with nonlocal nonlinearities. These results concern existence of blowing up solutions, as well as their singular behavior (blowup sets, rates and profiles). We then compare them with the corresponding results in the local case, and we show that the two types of problems exhibit "dual" blowup behaviors.

CHRISTIANSEN, Peter L (Department of Mathematical Modelling, Technical University of Denmark, Denmark)

Nonlinear waves in media with long range interactions

Long range interactions occur in media with dipole-dipole interactions in the molecular structure e. g. We study the propagation of localized nonlinear waves in a class of media with such interactions. Analytical results obtained by the method of collective coordinate are compared to direct numerical solutions of the dynamical equations. This is a joint work with Yu B Gaididei, M Johansson, J Juul Rasmussen, V Mezentsev, K Oe Rasmussen, D Usero, D Henriksen, and L Vazquez.

DAI, Hui-Hui (City University of Hong Kong, Hong Kong)

Existence of kink waves in a modified Mooney-Rivlin elastic rod

In literature it was conjectured that kink waves may propagate along an incompressible hyperelastic rod. However, exactly for which type of material and under which physical conditions such waves can arise is not known yet. Also, an analytical description is not available. Here, to resolve these issues we study travelling waves in a modified Mooney-Rivlin material. A system of ordinary differential equations arises. Two important features are: (a) The critical points are governed by a sixth-order polynomial equations involving four physical parameters. (b) There are no or one or two singular lines. Here, we shall concentrate on the non-singular case. To consider the global bifurcation of the critical points in a four parameters space imposes a mathematical challenge. This is successfully resolved by using the concepts of normal forms and universal unfoldings in the singularity theory. As a result, we can prove conclusively that kink waves can indeed arise and a complete analytical description is also provided.

ENGELBRECHT, Juri (Institute of Cybernetics, Estonian Academy of Sciences, Tallinn, Estonia)

Solitonic structures in KdV-based higher-order systems

Wave propagation in microstructured materials is studied using a KdV-type nonlinear evolution equation. Due to the microstructure, nonlinear effects are described by a quartic elastic potential and dispersive effects by both the third- and the fifth-order space derivatives. The problem is solved numerically under harmonic initial condition. For nondispersive materials, the quartic elastic potential, compared with that of the second order (KdV) one, leads to the formation of two additional discontinuities in the harmonic initial waveprofile. This together with the additional dispersive effect is the reason for emerging complicated solitonic structures (train of solitons, train of negative solitons, multiple solitons) depending on the values of dispersion parameters. Chaotic motion results if both the third- and the fifth-order dispersion parameters take the small possible values. This is joint work with Andrus Salupere.

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MSP-014
MSP-015
MSP-016

HILL, Sandra (Keele University, UK)

Nonlinear waves in a coated elastic half-space

We consider propagation of nonlinear travelling waves in a coated elastic half-space. To simplify analysis, we assume that both the coating and half-space are made of neo-Hookean materials with shear moduli $\hat{\mu}$ and μ , respectively. We use $r = 1 - \hat{\mu}/\mu$ as a tuning parameter with the limit $r \rightarrow 0$ corresponding to an uncoated half-space. When $r = O(1)$, the bonded structure is strongly dispersive and it is well-known that it can support a nonlinear sinusoidal wave (i.e. a Stokes wave). We focus our attention on the case when r is small (so that the coated half-space is weakly dispersive) and we look for a multiple-mode travelling wave solution in which the displacement field takes the form of a Fourier expansion. The system of evolution equations for the amplitudes of Fourier modes is derived and its solutions are discussed. This is a joint work with Y. Fu.

KAWAHARA, Takuji (Kyoto University, Japan)

Wave propagations in lattice models for nonlinear elastic structures

Generations and propagations of nonlinear waves in some nonlinear periodic structures composed of elastic elements are investigated in terms of discrete lattice models. Considered models are a Toda type lattice with external linear elastic force, a lattice composed of an array of dumb-bells, and a lattice including damping effect, which describe, respectively, a periodic structure like honeycomb, so-called Timoshenko beam, and certain visco-elastic materials. Discrete lattice equations are solved numerically and obtained results for evolutions of solitons and envelope solitons are discussed in comparison with the continuum approximations.

KOSEVICH, Yuriy A (Max Planck Institute for Physics of Complex Systems, Dresden, Germany)

Dissipative interaction and anomalous surface absorption of bulk elastic waves at a two-dimensional defect in a solid

The effect of bulk and surface dissipation on resonant interaction of bulk elastic waves with a thin elastic layer (2D defect) sandwiched in a solid is considered. We predict an extreme sensitivity to the dissipative losses, especially to the bulk ones, of the resonant interaction of the elastic waves with the 2D defect. The coefficients of the resonant transmission and reflection of the transverse wave at the 2D defect are derived with an account for the bulk and surface dissipation. We show that almost total reflection of the transverse elastic wave at resonance with the quasilongitudinal leaky wave at a 2D defect, described earlier without an account for the dissipation, occurs only in the limit of extremely weak dissipation. In this limit the coefficient of surface absorption R_s of the incident wave is small and is proportional to the bulk viscosity and thermal conductivity of the solid, but is inversely proportional to the square of the frequency. We show that almost total resonant reflection of the transverse wave at the 2D defect can be changed into almost total transmission by relatively weak bulk absorption. Anomalous surface absorption of the transverse acoustic wave, when R_s reaches its maximal value 0.5 and which is caused by resonant dissipative interaction with the leaky elastic wave, is predicted for the case of "intermediate" bulk dissipation.

KOSIŃSKI, Witold (Center of Mechanics and Information Technology, SPOKoMM, IPPT PAN, Poland)

Thermomechanical coupled waves in nonlinear medium

To deal with thermal wave propagation in a deformable continuum a gradient internal state variable approach has been recently developed by the first author. The approach leads to a modified Fourier law and admits wave like heat conduction governed by a system of quasi-linear hyperbolic equations. The present model accounts for a strong thermomechanical coupling and a temperature dependent speed of thermal waves.

Within this model nonlinear thermomechanical coupled wave propagation is analyzed qualitatively and quantitatively. A numerical scheme is developed to solve initial-boundary value problems in finite domain. A comparison between obtained numerical solutions and experimental results observed for selected media in the relevant range of temperatures, is made. This is a joint work with Kurt Frischmuth.

MAUGIN, Gerard A (Universite Pierre et Marie Curie, Laboratoire de Modelisation en Mecanique, Paris, France)

Soliton-complex dynamics in strongly dispersive media

The concept of "soliton complex" in a nonlinear dispersive medium is formulated. It is shown that interacting identical topological solitons in the medium can form bound soliton complexes which move without radiation. This phenomenon is considered to be universal and applicable to various physical systems issued from microstructured elasticity and magnetism. The soliton complex and its "excited" states are described analytically and numerically as solutions of nonlinear dispersive equations with the fourth and higher-order spatial or mixed derivatives. The dispersive sine-Gordon, double and triple sine-Gordon, and piecewise models are studied in detail. Mechanisms and conditions for the formation of soliton complexes, and peculiarities of their stationary dynamics are investigated. A phenomenological approach to the description of the complexes and the classification of all possible complex states are proposed. Some examples of physical systems where the phenomenon can be experimentally observed are briefly discussed. This is a joint work with Mikhail M. Bogdan and A.M.Kosevich.

MAUGIN, Gerard A (Universite Pierre et Marie Curie, Laboratoire de Modelisation en Mecanique, Paris, France)

Shock-wave and phase-transition-front structure by means of Eshelbian mechanics

The formulation of solid mechanics entirely on the material manifold - and not in physical space - has demonstrated its full power while dealing with local structural rearrangements of matter in solids. The Eshelby material stress is of paramount importance in that framework. Here it is shown that a full thermomechanics of the progress of discontinuity surfaces of the shock-wave and phase-transition types, emerges in such a framework, including the expression of the entropy growth which is directly related to the power expanded by the driving force (due to the Eshelby stress) on the surface. Both in fact follow from the jumps of a single scalar generating function and of temperature. The relationship with the dissipative forced motion of a solitonic structure is demonstrated.

MAYER, Andreas P (Institut fuer Theoretische Physik, Universitaet Regensburg, Germany)

On the stability of surface acoustic solitary waves in coated elastic media

Coating a planar surface of a homogeneous elastic halfspace by a thin film gives rise to dispersion of Rayleigh waves that, together with the second-order nonlinearity of the substrate, leads to the existence of surface acoustic solitary pulses. Their shapes are computed and their stability with respect to small changes of their initial conditions and to collisions with each other is investigated numerically. The existence of sagittally polarized envelope solitons and gap solitary waves in the case of a periodically structured film is demonstrated, and a numerical method is presented to investigate stability properties of the latter. This is a joint work with C Eckl, A S Kovalev, G A Maugin, and J Schoellmann.

PASTRONE, Franco (Department of Mathematics, University of Torino, Italy)

Non-linear waves in solids with microstructures: Dissipation and amplification problems

We study the influence of dissipative constitutive relations for the microstructure on wave propagation, a phenomenon which may lead, in special situations, to somewhat unexpected results, such as a reservoir effect of the microstructure which may drive the amplification of deformation waves. Such effects are observed in seismic waves. In particular, we analyze models in which the microstructure can absorb or release energy depending on the amplitude of the incoming deformation wave, so that the material as a whole behaves as a dissipative material for small perturbations, while larger perturbations can be amplified. In the three-dimensional case, anisotropy in the distribution of the damages may induce a waveguide effect for the propagation of deformation waves.

PORUBOV, Alexey V (AF Ioffe Physico-Technical Institute of the Russian Academy of Sciences, Russia)

Strain solitons in an elastic rod embedded in external medium

We study the influence of the external medium on the propagation of nonlinear elastic longitudinal strain solitary waves (i.e., strain solitons) in a cylindrical rod by the examples of the sliding contact with an elastic medium and of the contact with viscoelastic medium. In the former case we find the similarity of the governing equation with the case of free surface rod. However, now the waves have phase velocity in an interval, determined by the elastic properties of the external medium, also, it defines the type of strain soliton (compression or tensile). In the latter case we obtain new governing nonlinear dispersive-dissipative equation with an appropriate input-output energy balance. As a result, this equation admits exact dissipative solitary wave solutions, which parameters are defined by the values of the coefficients of the equation. When dissipation is small enough an initially dissipationless strain solitary wave is shown to transform to a dissipative solitary wave with prescribed parameters. This is joint work with A M Samsonov.

POTAPOV, Alexander I (Mechanical Engineering Research Institute, Russia)

Nonlinear interactions of solitary waves in a 2D lattice

A square lattice consisting of pointwise particles is considered. The interactions between neighbouring particles are described by a cubic potential. The governing equations have been derived both for the discrete model and in the continuum limit. Evolution equation has been obtained for nonlinear quasi-plane waves in the lattice. A long-term evolution of 2D quasi-plane solitary waves is investigated. The development of periodic soliton modulation, in an unstable region, leads to formation of a 2D stationary wave. This process is accompanied by the radiation of a small amplitude plane soliton. Multisoliton solutions of the Kadomtsev-Petviashvili equation are analyzed using exact and approximate methods. This is joint work with I S Pavlov, K A Gorshkov, and G A Maugin.

POUGET, Joel (Universite Pierre et Marie Curie, Laboratoire de Modelisation en Mecanique, Paris, France)

Nonlinear modulation of wave packets in a shallow shell on an elastic foundation

Among a lot of fascinating nonlinear effects, there is great deal of interest in self modulation of a plane wave, or modulational instability (MI), which occurs in nonlinear dispersive media. Qualitatively a MI is the tendency for an amplitude of a modulated carrier wave to break into isolated structures or solitons. Energy originally resident in the carrier of the train wave or long pulse is gradually transferred, by nonlinear interaction, in the medium, into the spectrum side bands. As the side-band energy grows in amplitude, the modulated wave breaks up into a series of localised objects or envelope solitons. Composite structures formed by a singly or doubly shallow shell resting on a non-linear elastic foundation are wave guides that enable one to focus a high energy density in order that nonlinearities be excited. This class of elastic structures is an interesting candidate for the real observation of two-dimensional localised modes in elastodynamics. The purpose of the present work is to study the influences of the geometric dispersion, the prestress on the shallow shell and the material nonlinearity of the elastic foundation on the vibrations modes of the structure. The basic equations which govern the dynamics of the elastic structure are deduced from a variational principle. The analysis is restricted to signals which consist of a slowly varying envelope in space and time modulating a harmonic carrier wave. In the limit of low amplitude the coupled equations are solved by means of a reductive perturbation method. It is shown that the complex amplitude of the envelope is governed by a two-dimensional nonlinear Schrödinger equation coupled to two other amplitude equations associated with midsurface motion of the shell. The latter system allows us to study the modulational instability conditions leading to different zones of instability. The mechanism of the self-generated nonlinear waves in the elastic structure beyond the birth of modulational instability is numerically investigated on the original equations.

SAMSONOV, Alexander M (The Ioffe Institute of the Russian Academy of Sciences, Russia)

Bulk nonlinear elastic waves in inhomogeneous wave guides

Nonlinear elastic features of materials result in generation of new localized waves - bulk strain solitons even under short-run and weak reversible (elastic) loading. Based on theory of long nonlinear strain waves in wave guides a new physical phenomenon was established to exist, namely: elastic energy can be transferred along a wave guide by means of strain solitons without significant energy losses despite of absorption features of elastic material. Amplification (focusing) of the soliton was predicted and observed in a tapered rod as well as an asymmetric deformation of the focused pulse. An explicit relationship was obtained for the soliton amplitude vs cross section variations of the wave guide. Numerical simulations and a new visualisation programme were developed to study strain soliton evolution in various inhomogeneous and complex rods, composed of different insertion blocks or partially embedded in another elastic medium. Moreover, the propagation of a solitary wave in a wave guide having stochastic properties (e.g., due to roughness) was studied by means of direct Monte Carlo simulation. A set of distinctive characteristics of soliton to test an internal structure of a wave guide is proposed.

SAXTON, Ralph (University of New Orleans, USA)

On second sound at the critical temperature

We derive a physically justifiable model of heat conduction for rigid heat conductors based on an recent approach involving the gradient generalization of an internal state variable. The model accounts for observable phenomena in solid dielectric crystals, related to wave-like conduction of heat in certain ranges of low temperatures and a rapid decay of the speed of thermal waves close to a transition temperature value, at which the conductivity of the material reaches a peak. These are used to specify admissible forms of the constitutive equations and material functions involved. An analysis of weak and strong discontinuity waves is given in order to exhibit several main features of the proposed model. This is joint work with Witold Kosinski.

TRIMARCO, Carmine (University Of Pisa, Italy)

On a progressing phase transition front

A phase transition front in a solid may be viewed as a homothermal shock wave which transforms one phase into another while progressing. If the geometrical regularity of the two crystalline lattice sites is not affected across the front, the phase transition is said to be coherent. In the language of continuum mechanics, coherence addresses to geometrical compatibility conditions across the front. Such conditions address, in turn, to kinematical compatibility conditions for the motion of the lattice sites. The latter slightly differ from the classical kinematical conditions across a wave front. Hence, one is led to introduce the notion of full coherency.

BRÜHL, Martin (Universität Karlsruhe, Germany)

Reconstruction of inclusions with electrical impedance tomography

In electrical impedance tomography currents are applied to a two-dimensional body and the resulting voltages are measured on the boundary. The goal is to use these (overdetermined) boundary data to reconstruct information about the conductivity coefficient within the body.

It is known that these boundary data (the Neumann-to-Dirichlet operator) uniquely define piecewise smooth conductivities. This may correspond to the practical situation that a body consists of a number of inhomogeneities in a homogeneous background medium. We present a theoretical characterization of the domain of these inclusions which leads to a cheap numerical algorithm for the reconstruction of their domain.

CHENEY, Margaret (Rensselaer Polytechnic Institute, USA)

An asymptotic wave interpretation of sonar images

This talk considers the inverse problem of determining the shape and medium parameters of the seafloor from sonar data. First we review beamforming techniques and the Kirchhoff (high-frequency) approximation. Next we carry out a stationary phase calculation for various measurement configurations associated with side-scan sonar and pencil-beam sonar. These results provide an interpretation of the information content of sonar images. The pencil-beam sonar, in particular, allows reconstruction of the shape and acoustic impedance of the seafloor.

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MSP-017

NAGY, James (Southern Methodist University, Dallas, USA)

Resolution enhancement of CT images using spatially variant image restoration methods

Images obtained from computerized tomography (CT) systems can be corrupted by geometric distortions and severe streaking artifacts resulting, for example, from limited data, presence of opaque foreign objects, and motion of the patient. Image restoration techniques can be used to improve the resolution of these images, but numerical methods are difficult to implement efficiently due to the spatial variation of the resulting point spread function (PSF). In this talk, we describe a scheme for approximating the spatially variant PSF, and show that image restoration methods can be efficiently implemented with this approximation.

PIDCOCK, Michael (Oxford Brookes University, UK)

Image reconstruction in electrical impedance tomography

The inverse conductivity problem is interesting because it is quite simple to describe and yet is very challenging from a mathematical viewpoint and because it has a practical realisation in Electrical Impedance Tomography (EIT). EIT is being studied extensively with a number of medical and industrial applications in mind. In this talk I will describe an integral equation formulation of the image reconstruction problem for the inverse conductivity problem and some of the ways in which the approach can be developed to help EIT to become a practical reality.

SANTOSA, Fadil (Institute for Mathematics and its Applications, University of Minnesota, Minneapolis, USA)

Quantitative nondestructive evaluation using Eddy current methods

Eddy current method for is a nondestructive evaluation technique that uses EM fields at low frequency to probe the presence of damage. While the method is very effective in detecting damage, it is less successful in obtaining quantitative information about the damage. We study the illposed problem arising in attempting to perform quantitative nondestructive evaluation. We pose regularization strategies and investigate their effectiveness in numerical simulations.

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MSP-018

FRIGAARD, Ian (Schlumberger Dowell, Clamart, France)

Novel imaging-type problems arising in oilfield cementing

When cementing an oil well a number of imaging-type problems arise. For example, after the cement has set, acoustic logging techniques are used to determine the quality of bond between the cement and the formation. The mathematical problem arising here is quite similar to other classical imaging problems.

Non-classical imaging-type problems also arise before the cement has set. The fluids pumped, (muds, spacers, cement slurries), are non-Newtonian yield stress fluids and the flows are often either slow and/or uniaxial, resulting in non-differentiable minimisation problems. A regularisation method is used, similar to those used for image enhancement and reconstruction. For some of the flow problems this technique works well, whereas for others it fails miserably. A number of instructive examples are discussed.

SCHOISSWOHL, Armin (Industrial Mathematics Institute, Johannes Kepler University Linz, Austria)

Image matching as an example of an inverse problem in medical imaging

In medical imaging image matching algorithms are applied for the generation of compound images or the evaluation of comparative images of affected organs. Mathematically image matching results in the problem of determination of a transformation that matches two data sets. This transformation can be obtained as the minimizer of a nonlinear least squares functional. A multiscale strategy on the basis of wavelet decompositions of the data is used for the solution of the image matching problem. Numerical simulations with medical ultrasound data are presented.

VOGEL, Curtis R (Montana State University, USA)

Inverse problems in atmospheric optics

Assuming an "optically thin" atmosphere and an extended incoherent light source, an accurate model for recorded image data is $d = s[\phi] * f + \eta$, where f denotes the unknown object, η represents instrument recording error, $*$ denotes 2-D convolution, and the dependence of the point spread function s on the unknown phase, or wavefront, aberration is given by $s[\phi] = |\mathcal{F}(Ae^{i\phi})|^2$. Here A is a known aperture function, and \mathcal{F} denotes 2-D Fourier transform.

We will address (i) types of data that are sufficient to uniquely determine both f and ϕ , and (ii) numerical schemes to efficiently estimate f and ϕ from this data.

WEICKERT, Joachim (University of Copenhagen, Denmark)

Restoration methods in computer vision

We study relations between regularization and diffusion filtering in image processing. Regularization is regarded as single step implicit time discretization of a diffusion process. It is shown that iterated Tikhonov regularization handles noise better than noniterated. We argue that the Perona-Malik filter, a popular forward-backward diffusion process, acts total variation-diminishing, and we present a novel regularization which can be formulated as energy minimization. Experiments on noisy real-world images illustrate the restoration properties of Tikhonov and total variation restoration for the noniterated and iterated case. This is joint work with Otmar Scherzer.

ADAMS, Brent L (Carnegie Mellon University, Department of Materials Science & Engineering, Pittsburgh, USA)

Continuum dislocation fields at grain boundaries in deformed polycrystals: An experimental approach

Orientation imaging microscopy is used to study the curvature of the crystal lattice in the vicinity of grain boundaries in deformed aluminum polycrystals. The curvatures observed are interpreted in terms of the geometrically-necessary dislocation (GND) content required for their support in the lattice. Estimates of the local dislocation tensor field are obtained as a function of distance from the grain boundary. At plastic strain levels of 0.1 the density of GNDs is observed to peak at grain boundaries of all types, suggesting a pileup-like behavior. At larger strains of 0.3 a variety of behaviors are observed, dependent upon the crystallographic character of the grain boundary. These observations have been correlated with the evolution of character of the grain boundary during deformation. The data suggest that grain boundaries may selectively absorb (or emit) GNDs in a manner that reduces the overall energy of the system. The implications for grain boundary engineering are examined.

BALL, John M (University of Oxford, UK)

Models for surface relaxation

The different atomic environment of atoms near a free surface of a crystal typically leads to a localized deformation near the surface. The predictions for such surface relaxation are explored for models based on a free energy function depending on a finite number of derivatives $D^{(i)}y$, $1 \leq i \leq N$, of the deformation y . It is shown that second-gradient theories ($N = 2$) do not in general predict surface relaxation, but that if third derivatives are included ($N \geq 3$) then surface relaxation can be predicted. Various explicit models are analyzed using variational methods and phase-space techniques. A study is also made of kink solutions joining two stable phases and of the interaction of these with surface relaxation, both in a static and dynamic context.

This is joint work with K Huang (Oxford) and E K H Salje (Cambridge).

BOUCHITTE, Guy (University of Toulon, France)

Singular perturbations related to a potential degenerated at infinity: Applications to nucleation and free discontinuity problems

We present recent results about the asymptotic of a two phases Cahn and Hilliard fluid in the case where the liquid phase ratio is small. By rescaling we are led to a situation where the second well of the potential W is achieved at infinity (precisely $W(u) \sim |u|^p$ with $p < 1$). We show that the equilibrium solutions concentrate and converge to a purely atomic measure (droplets) whose energy depends on the mass of each atom. In a second part, we apply our analysis to a higher order problem and obtain a smooth approximation of the Mumford and Shah functional.

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CHIPOT, Michel (Institut fuer Mathematik, Universitaet Zuerich, Zurich, Switzerland)
Computing microstructures

We present recent results regarding the computation of microstructures. Some practical and theoretical issues will be considered.

DESIMONE, Antonio (MPI for Mathematic in the Sciences)

Energetics of fine domains

In the last few decades, new mathematical tools have become available for the analysis of minimization problems involving non-convex free-energies. These advances have shed some new light on the behavior of a variety of physical systems exhibiting domain structures, and on their response to external actions (forces, electromagnetic fields, etc.). Examples range from ferroelastic solids (in particular, shape memory alloys) to ferromagnetic and ferroelectric materials (in particular, solids with strong electro- or magneto-elastic coupling). In this talk, striped domain patterns observed in liquid crystalline polymers are discussed, showing that the emergence of domain structures, and the success of the mathematical techniques for their analysis are not peculiar to crystalline solids.

FONSECA, Irene (Department of Mathematical Sciences, Carnegie Mellon University, Pittsburgh, USA)

Relaxation results for constrained variational problems

Several interesting questions in materials science require a good understanding of constrained variational problems. The study of equilibria for liquid crystals and magnetostrictive materials motivates the search for relaxed energies under Lipschitz manifolds constraints, leading to the notion of tangential quasiconvexification. The analysis of problems related to phase transformations for solid materials involving change in chemical composition asks for existence of minimizers and characterization of optimal designs when the underlying fields are subject to fixed volume fraction constraints. These are some of the issues in relaxation theory for constrained problems that will be addressed in this talk.

FRIESECKE, Gero (Mathematical Institute, University of Oxford, UK)

Existence theorems for quantum many-body systems via variational methods

The nonlinear simplifications of "exact" N-body quantum mechanics (density functional theory, the Hartree-Fock equations, the Configuration-Interaction equations) have an enormous physics and chemistry literature, but few rigorous results. Recent progress includes a proof of existence of solutions and integer quantization of charge for the CI equations of atoms and molecules; as special cases one recovers the basic existence theorems of Zhislin in N-body quantum mechanics (infinite rank CI) and of Lieb-Simon in Hartree-Fock theory (rank-N CI) in a unified and natural way.

GREENBERG, James M (Carnegie Mellon University, Pittsburgh, USA)

Antiplane shear flows in visco-plastic solids exhibiting isotropic and kinematic hardening

The authors consider antiplane shearing motions of an incompressible visco-plastic solid. The particular constitutive equation employed assumes that the stress tensor has an "elastic" component and a component which can exhibit hysteresis. The model exhibits both "kinematic" and "isotropic" hardening. Our results consist of a set of energy type estimates for the resulting system, L_2 contractivity estimates for the solution operator, and finally an analysis of the approach of our system to a "rate independent" model as a distinguished parameter describing our flow rule approaches zero. We also include some computational results for simple piecewise constant data.

KINDERLEHRER, David (Carnegie Mellon University, Pittsburgh, USA)

Grain boundary energy and evolution

Most technologically useful materials are granular in nature, consisting of small single crystal grains separated by surface, the grain boundaries. The emerging discipline of grain boundary engineering has as its goal the optimization of the surface properties to enhance lifetime, durability, and more specific material properties. A first step in optimizing properties is the determination of the grain boundary energy. We have begun development of multiscale/statistical methods for this purpose. Here we describe their application in several test cases. There are a number of surprises. If time permits we shall discuss evolution. This work is part of the Mesoscale Interface Mapping Project, an NSF/MRSEC.

KOWALCZYK, Michał (Carnegie Mellon University, Pittsburgh, USA)

Dynamics of single spikes in the Gierer-Meinhardt system

The Gierer-Meinhardt system is one of the most common models for a biochemical reaction of the activator-inhibitor type. In this talk I will present some recent, rigorous results concerning the dynamics of single spikes in the Gierer-Meinhardt system as well as its shadow system. In both cases we derive a system of ODE's which governs the motion of the spike. Analysis of the reduced dynamics shows that, contrary to our original expectations, the shadow system may not be a good approximation of the full system even if the diffusion of the inhibitor approaches infinity while the diffusion of the activator approaches 0. In particular the stability of the spike is not preserved after passing to the limiting, shadow problem.

This is joint work with Xinfu Chen.

KRISTENSEN, Jan (Mathematical Institute, University of Oxford, UK)

Quasiconvexity and Young measures

Under favourable growth conditions a Young measure minimiser always exists. In this talk I discuss properties of Young measure minimisers and smoothness properties of quasiconvex envelopes. Some of the results have been obtained in collaboration with John Ball and Bernd Kirchheim, Georg Dolzmann, and Petr Plechac.

LEO, P H (University of Minnesota, USA)

The energy of semicoherent interfaces

A model for the energy of a semicoherent interface between any two arbitrary crystal planes is presented. The interface is separated into coherent regions and defect regions, where the defects compensate for the misfit between the two crystals. The relaxed energy of the interface after separation is given by the weighted average of the energy of the individual regions. Thus given any two Bravais lattices with arbitrary lattice constants, one can find the set of planes that yield the best fitting, low energy interfaces. Calculations are presented to find these low energy plane pairs in a face centered cubic/body centered cubic system. The results are consistent with experimental data, though the agreement is far from exact.

LIU, Chun (Penn State University, USA)

Some dynamic problems in the theory of liquid crystals

The term liquid crystal refers to the intermediate phases between the solid and the isotropic liquid phase. In this talk, we will discuss existence, regularity and stability of the solutions of several dynamic systems modeling different types of liquid crystals. For instance, the hydrodynamic theory of the nematic liquid crystals established by Ericksen and Leslie in 60's and the recent model proposed by Weinan E for the Smectic A liquid crystals. We will also present some numerical simulations for the Ericksen-Leslie system. The emphasis is the coupling between the flow velocity and the alignment of the molecules.

Part of the talk is joint works with Fang-Hua Lin and Noel Walkington.

LUCKHAUS, Stephan (Universitaet Leipzig, Germany)

Stefan problems as gradient flows for the entropy Stefan problems as gradient flows for the entropy

Stefan Problems with and without surface tension can be viewed as gradient flows for the entropy. This is particularly useful for systems of heat and mass diffusion. A big problem for the theory though is the nonappearance of mushy zones for surface tension tending to zero.

LUSKIN, Mitchell (University of Minnesota, Minneapolis, USA)

Stability of microstructure in Martensitic crystals

We present a theory for the stability of simply laminated microstructure in martensitic crystals. The analysis of stability becomes more difficult for crystals with phase transformations which undergo a greater loss of symmetry (and hence have more variants) since the crystal then has more freedom to deform without the cost of additional energy. In joint work with Pavel Bělík, we have recently given an analysis for all of the tetragonal to monoclinic transformations (which have four variants); and in joint work with Kaushik Bhattacharya and Bo Li, we have given an analysis for a cubic to orthorhombic transformation (which has six variants). We have shown for these transformations that the simply laminated microstructure is stable, except for special lattice constants at which the simply laminated microstructure is not stable.

MILTON, Graeme W (Department of Mathematics, University of Utah, USA)

Bounding the stress-strain relation of non-linear composites

Considerable work has been done on bounding the elastic energy of non-linear composites. Yet the stored elastic energy is a difficult quantity to measure, requiring one to integrate the work done to achieve a given deformation. From a practical viewpoint it may prove more important to bound the average stress given an average strain since these are direct physically measurable quantities. In this lecture we show how this can be done. The problem is reduced to bounding a certain non-convex scalar valued function and the same methods that have been developed to bounding energies can be directly applied to bounding this function. We also discuss the question, both in the non-linear and linear case, of what microstructures have optimal stress-strain combinations. Such optimal microstructure are important in optimal design for guiding stress to desired locations.

This is joint work with Sergei Serkov, Alexander Movchan, and Valery Smyshlyaev.

NOVICK-COHEN, Amy (Technion-IIT, Israel)

Wetting, prewetting, and the driving force paradox

A system of Allen-Cahn/Cahn-Hilliard equations is considered as a diffuse interface model for microstructural evolution in the framework of simultaneous phase-separation and ordering in binary alloys. In the neighborhood of the tricritical point, analysis of the limiting equations of motion yields the resolution of a longstanding driving force paradox. Issues of wetting, prewetting, and adsorption are addressed, and the possibility of dynamic inhibition of complete wetting is noted. This is a joint work with J W Cahn.

ORTIZ, Michael (Graduate Aeronautical Laboratories, California Institute of Technology, USA)

Kinetic roughening and coarsening in thin films

We present a phenomenological continuum model of film growth based on a series expansion of the deposition flux in powers of the profile gradient, consideration of the energetics of the film/substrate interface, and the enforcement of Onsager's reciprocity relations. The interfacial term, which operates at very small thicknesses, is nonconservative and breaks the $\pm h$ symmetry of the remaining terms in the kinetic equation. By virtue of this term, very thin flat films are predicted to be stable within an appropriate range of parameters, and to lose stability and become rough at a well-defined critical thickness. This instability effectively provides a island nucleation mechanism. For thick films, the rate processes envisioned in the model favor a characteristic slope for the film profile, a feature which is in keeping with observation for a number of systems including YBCO films. The enforcement of reciprocity ensures the existence of a kinetic potential and enables the use of direct methods of the calculus of variations. Within this framework, we provide an explicit construction for the coarsening of the film profile based on a sharp interface approximation. The construction predicts characteristic exponents for the evolution of grain size and film roughness which are in close agreement with the observational evidence for YBCO. The predictions of the construction are also born out by numerical tests.

OTTO, Felix (University of California at Santa Barbara, USA)

Thin film ferromagnets

A soft ferromagnet is placed in an external magnetic field. The sample is a thin film in plane with the field. It is observed that the sample splits into a few 2-d domains, where the magnetization varies smoothly, separated by "walls". We derive predictions of the well-accepted 3-d dimensional micromagnetic model w. r. t. the position of these walls. Our method is a rigorous renormalization of the variational problem in the thin film limit. We also present numerical analysis of the renormalized problem. This is joint work with Antonio DeSimone, Bob Kohn, and Stefan Mueller.

PEDREGAL, Pablo (Universidad de Castilla-La Mancha, Spain)

Relaxation in magnetostriction

The analysis of the magnetostriction functional, where the interaction between elastic and magnetic properties of materials is taken into account, is undertaken under important simplifying assumptions which are close to the typical linear theories of magnetostriction. The key ingredient of this analysis is a local version of the original nonlocal optimization problem that allows for a formulation in terms of Young measures. Some minimizing configurations can be recovered from the associated relaxed functional.

PIRONNEAU, Olivier (University of Paris 6, France)

Application of automatic differentiation of computer programs to PDEs

Automatic differentiation of program (AD) has been around for some years (ADOLC, ADIFOR, ODYSSEE...) but it remained a tool for specialist till some realized for themselves that it could be done very simply using operator overloading in C-classes or FORTRAN90 structures. The basic idea is that a computer program can be differentiated with respect to any variable because each line of the program can be differentiated symbolically. There are two ways to implement AD, the forward mode and the backward mode, corresponding to the computation of derivatives by the chain rule as the partial derivative of the Lagrangian, i.e. depending whether the lines of the computer program are seen as explicit formula for the constraint variables or as constraints on all variables. The fact that one obtains automatically and simply such derivatives the moment the computer program for solving a PDE is written, has far reaching practical consequences for sensitivity analysis and optimization which we will illustrate on a few examples.

SERRE, Denis A G (Ecole Normale Supérieure de Lyon, France)

Vorticity growth in swirling flows

One considers the swirling flow of an incompressible perfect fluid between two cylinders. The data may be periodic in the z -variable. One shows that under very general assumptions, the amplitude of the vorticity grows at least linearly in time. Indeed, this growth either holds on a set of Hausdorff dimension ≥ 2 , or is super-linear.

TA'ASAN, Shlomo (Carnegie Mellon University, Pittsburgh, USA)

Multiscale simulations of grain boundaries

The mechanical behavior of polycrystalline materials depends on their microstructure which includes grains, grain boundaries, dislocations, voids and impurities. The prediction of material strength is important for many applications and it depends to a large extent on grain size, the smaller the grains the higher the strength of the material. The grain size distribution is, therefore, a quantity of importance from both an engineering and a scientific viewpoint. Simulation techniques can be used to address this problem. In this talk we focus on efficient multiscale numerical simulation for studying the dynamics of a large network of grains in two dimensions. Grain boundaries in our model satisfy parabolic PDE's, i.e., they move by mean curvature, and triple junctions satisfy the Herring condition. Simulations involving thousands of grains and the evolution of their boundaries will be presented. In particular, the evolution of grain size distribution will be discussed.

This is a joint work with David Kinderlehrer and Florin Manolache.

TARTAR, Luc C (Carnegie Mellon University, Pittsburgh, USA)

The applications of H-measures and their variants to partial differential equations from continuum mechanics and physics

In 1976/77, I successfully proposed a new method for the analysis of the nonlinear partial differential equations of continuum physics based upon ideas in the theories of homogenisation and compensated compactness that I had previously developed jointly with Francois Murat. The "Compensated Compactness Method", as I termed this method, generalised all the previous known methods involving, for example, convexity, Young measures, monotonicity and compactness. Even so, more powerful tools were soon demanded. In the light of experience gained with the advantages and limitations of my method, as well as with more recent ones, including that by P-L Lions and called by him the concentrated compactness method, which name incidentally has apparently caused some unfortunate confusion, I was able to improve the scope of compensated compactness by the introduction in 1986/87 of H-measures. (These measures were later independently introduced by Patrick Gerard, but under a different name.) Although H-measures provide the first mathematical proof that in the limit of infinite frequency waves behave like particles, it is necessary in certain problems to use a variant employing characteristic lengths. The same approach was independently introduced by Patrick Gerard, with the techniques of P-L Lions and Thierry Paul appearing a little afterward. The talk will describe applications from continuum mechanics, for which the use of these or other variants of H-measures becomes crucial.

TRUSKINOVSKY, Lev (University of Minnesota, USA)

Mechanical behavior of discrete systems with multi-stable elements

Modern technology operates at a scale where complexity of the mechanical behavior can only be achieved if a "mechanism" is integrated into the material at the molecular level. Thus, "smart" materials are characterized by a multi-stable response at the microlevel which means non-convexity of the elastic energy of a representative snap-spring. This leads to a nontrivial relation between discrete and continuum models: the corresponding discrete problems possess multiple local equilibria with the energy landscape which may be infinitely "bumpy". As a result, the system can get locked, which leads to the hysteretic behavior. In dynamics, multi-stability at the discrete level also raises interesting problems. In particular, it turns out that the homogenization of a purely mechanical discrete system with bi-stable elements must necessarily be thermodynamical.

WALKINGTON, Noel J (Carnegie Mellon University, Pittsburgh, USA)

New variational principles for approximating parabolic PDEs

We illustrate how some remarkable new variational principles can be used for the numerical approximation of solutions to certain (possibly degenerate) parabolic partial differential equations. One remarkable feature of the algorithms presented here is that derivatives do not enter into the variational principles, so, for example, discontinuous approximations may be used for approximating the heat equation. We present formulae for computing a Wasserstein metric which enters into the variational formulations.

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BISCARI, Paolo (Milan University, Italy)

Curvature effects on nematic surface viscosity

Boundary surfaces influence the dynamic as well as the static properties of nematic liquid crystals. Derzhanski and Petrov (Acta Phys. Pol., A55 (1979), 747) first proposed a phenomenological dynamic condition to be imposed at the boundaries, introducing a *surface viscosity* γ_s , different from the usual bulk viscosity η . Recently, Durand and Virga (to appear in Phys. Rev.E (1999)) proved the validity of that condition in the case of a nematic delimited by a planar surface, also determining how γ_s depends on the anchoring angle ϑ_s . We prove that the surface viscosity depends also on the curvature of the surface and apply this result to determine the dynamic boundary conditions to be imposed on a liquid crystal confined to a cylindrical tube.

CALDERER, Carme (Pennsylvania State University, USA)

Mathematical modeling of Chiral Smectic A liquid crystals

We develop the point of view that Smectic A liquid crystal configurations are periodic solutions of an *extended nematic* theory. Accordingly, we identify the physical mechanism responsible for the symmetry breaking of the nematic causing the nucleation of the smectic A phase. We compare the outcome of such modeling approach with the well-known theories of the smectic A-nematic phase transition due to Landau, de Gennes and Lubensky. In particular, our studies yield a good understanding of the analogies and discrepancies with the modeling of superconductivity. In the case of chiral liquid crystals, we apply our model to the study of "Twist Grain Boundary" phases. Some of the topics presented here are joint work with Patricia Bauman, Chun Liu, Daniel Phillips, Lev Truskinovsky and Karl Voss.

GARTLAND, E C (Kent State University, USA)

Numerical modelling of defects and fine structure in confined liquid crystal systems

There has been a high degree of interest for some time now in equilibrium structures and defects of the orientational properties of liquid crystals in confined geometries. We report on a detailed numerical study of such phenomena in spherical droplets subject to radial "strong anchoring" boundary conditions and modeled by the Landau-de Gennes tensor-order-parameter free-energy model. Within the class of axially symmetric solutions, we find two familiar core structures: a radial point defect (or "hedgehog") and a small ring/loop disclination. In addition, we have found a new configuration, which is metastable within this symmetry class. Bifurcation and phase diagrams indicate how these three solutions, relate to one another.

LESLIE, Frank M (University of Strathclyde, Glasgow, UK)

Flow induced switching in a bistable device

Recently Dozov, Nobili and Durand have proposed a new type of bistable nematic liquid crystal display device, capable of very fast switching. The device differs from other recent proposals for bistable nematic displays in that it uses simple planar anchorings of different strengths at the plates. The device comprises two equilibrium states, one uniform and the other a π -twist, the alignment in both parallel to the plates. Switching between these states can be achieved using an electric field, straightforwardly from twist to uniform, but by exploiting the induced backflow for the reverse. Mathematically we endeavour to model such switching with backflow using continuum equations. Initially our efforts focus upon the transition from the uniform to bend state, and thereafter examine the completion to a π -twist. Different forms of the surface anchoring are considered.

STEWART, Iain W (University of Strathclyde, Glasgow, UK)

Layer undulations in finite samples of Smectic A liquid crystals subjected to uniform pressure and magnetic fields

This work derives theoretical results for finite samples of smectic A liquid crystals subjected to both a uniform pressure perpendicular to the smectic layers and a magnetic field applied in the plane of the layers or perpendicular to them; the special case of a uniform pressure with no field present is also considered. Criteria for suitable boundary conditions are derived for general finite sample geometries. Various critical field strengths are discussed in relation to the resulting 'grid-like' smectic layer undulations which arise as solutions to the governing equation. A comparison is drawn with known results for infinite samples.

GIBBON, John D (Imperial College, London, UK)

The theory of vorticity dynamics in the three-dimensional Euler and Navier-Stokes equations

We address the problem of how the direction of vorticity affects both 3D Euler and Navier-Stokes isotropic turbulence. In the context of the NS equations we study why the vorticity accumulates on 'thin sets' such as quasi-one-dimensional tubes and quasi-two-dimensional sheets. Taking our motivation from the numerical work of Ashurst, Kerstein, Kerr and Gibson (1987), who observed that the vorticity vector ω aligns with the intermediate eigenvector of the strain matrix S , we study this problem using the variables $\alpha = \frac{\omega \cdot S\omega}{\omega \cdot \omega}$ $\chi = \frac{\omega \times S\omega}{\omega \cdot \omega}$. This introduces the dynamic angle $\phi(x, t) = \arctan(\frac{\chi}{\alpha})$, which lies between ω and $S\omega$. For the Euler equations a closed set of differential equations for α and χ is derived in terms of the Hessian matrix of the pressure $P = \{p_{,ij}\}$. In collaboration with R. Kerr and B. Galanti, we have studied these equations using Kerr's 1993 singularity data. For the NS equations we discuss the role of the Burgers vortex and shear layer as the natural equilibrium solutions of the $\alpha - \chi$ equations. In a broader context we also study new columnar type stretched vortex solutions of the 3D NS equations which extend the Burgers solutions to those where the vorticity is no longer axial. These stretched vortices have a rich internal spatial structure the dynamics of which is linked to the pressure Hessian, which is a global quantity.

KAMBE, Tsutomu (University of Tokyo, Japan)

Vortex structures and statistics of turbulence

Fully developed turbulence is structured with a number of intense elongated vortices, and it is considered that statistical laws in turbulence is related deeply to such structures. Bearing these in mind, a simple model of turbulence statistics is proposed, which brings about probability density functions for longitudinal and transversal components of velocity difference when statistical averages are taken to ensure isotropy and homogeneity for an ensemble of strained vortices. It is found that the probability functions tend to close-to-exponential forms at small scales and that velocity structure functions show scaling behaviors with the scaling exponents close to those known in the experiments and direct numerical simulations. Furthermore, partial differential equations governing transition of the probability functions at different spatial scales are considered.

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IGNATYEV, Alexander O (Institute for Applied Mathematics and Mechanics, Donetsk, Ukraine)

Stability of permanent rotations of rigid body containing liquid

Consider rigid body with fixed point. It has an ellipsoidal cavity with ideal incompressible similar fluid performing turbulent rotation under following assumptions: gyration ellipsoids of fluid and rigid body are coaxial but barycenters of fluid and rigid body are inconsistent with fixed point.

From applications point of view one of the most interesting motions of this mechanical system is permanent rotation of rigid body around the principal axis containing barycenter and permanent rotation of fluid, as rigid body, around the same axis with the same angular velocity. Necessary and sufficient conditions of stability of such motion are obtained.

IGNATYEV, Andrey A (Donetsk State University, Donetsk, Ukraine)

Research of the motions of the rigid body

We obtained the algorithm of the stability research of permanent rotating heavy rigid body which has fixed point with ellipsoidal cavity, completely filled of ideal liquid which performs homogeneous rotational motion. In this paper on the base of this algorithm the programme for personal computer on the programming language "Pascal" was created. This is a joint work with A Ya Savchenko.

ILJUKHIN, Alexander A (Pedagogical institute, Taganrog, Russia)

Stability of the plain vibrations of two rigid bodies, connected with elastic rod

The artificial satellite of the Earth was considered as a system of two rigid bodies connected by an elastic rod. It was supposed that the system can make nonlinear oscillations around the center of masses. In particular the elastic rod makes the finite elastic displacements. The positions of a relative equilibrium of a system with varying geometry were found. In dependence on parameters of a system the axes of a rod in a position of an equilibrium can have some various forms that determines also angular positions of a system. The stability on some of variables (angular coordinates and characteristics of rod's geometry) was investigated for possible forms of an equilibrium in dependence on parameters of an orbit of the satellite and dynamic characteristics of a system. The areas of stability of a relative equilibrium of the satellite were constructed.

ILJUKHIN, Alexander A (Pedagogical institute, Taganrog, Russia)

Nonlinear phenomenons in one-dimensional theory of elastic rods

With the help of the asymptotic expansion on a relative thickness of a rod and variational method of Washizu the equations of the one-dimensional theory of finite displacements of elastic rods were constructed. In the case of deformation of rod only by ends moments an exact solution of the nonlinear equations of bending and torsion were reduced and dependencies of force and geometric characteristics on arc coordinate were obtained. Nonlinear equations for the definition of rod's axes displacements were integrated. The classification of the equilibrium forms of a rod in dependence on its parameters and the changes of a cross-section along its axes was given.

ILJUKHIN, Alexander A (Pedagogical Institute, Taganrog, Russia)

Vibrations of the rigid body on the elastic rod in airflow

Equilibrium and oscillations of a symmetrically streamlined rigid body was considered. The various cases of body strengthening and initial form of a rod were studied. The configurations of a system were found at a stationary flow. The stability of equilibrium was investigated. The methodical instructions for identification of aerodynamic parameters and accuracy control of offered dependancies of aerodynamic forces on velocity of a flow and geometry of a system were developed. With the aim of system sensitivity magnification to a velocity of a flow changes the rather thin elastic rods with a variable rigidity on bending were considered. It leads to necessity of finite elastic displacements of a system studing. The equations of nonlinear oscillations were reduced and the self-oscillating conditions were found.

KONONOV, Jury N (Donetsk State University, Ukraine)

On stability of unrestricted motion of the system containing connected rigid bodies with liquid filling

The motion of an elastic body with liquid filling in resistant medium is simulated by a system of elastic connected bodies with cavities containing liquid. The motion equations in resistant medium for a system of n-rigid bodies with cavities completely filled with viscous liquid are obtained. The stability of uniform rotations and rectilinear motion in resistant medium for a system of two rigid bodies connected by the elastic hinge and containing a viscous liquid is investigated.

KONOSEVICH, Boris I (Donetsk Institute of Applied Math and Mechanics, Ukraine)

Construction of the averaged equations for translational movement of the axially symmetric projectile

The asymptotic method of small parameter is applied to the system of 11 differential equations of motion of the shell. With the use of the second order approach solution of the equations of the angular motion the partially averaged equations of the progressive motion are obtained. These equations don't include addendums whose oscillating frequency equals to the higher frequency of the angular oscillations. It allows to compute the shell trajectory enough correctly ensuring the great economy of the computer time. The theoretical estimate of the error of the partially averaged equations is given and the computer experiments are carried out.

SAMSONOV, Vitalii (Lomonosov Moscow State University, Institute of Mechanics, Russia)

Computer modeling of continuum influence upon a rigid body

The teaching-methodical complex, intended for studying the properties of various dynamical models of the motion of a body under nonlinear effect of a resisting medium, is described. It is used to find, research and demonstrate the most typical modes of behaviour (self-oscillations, resonance, bifurcations and catastrophes, stochastic modes, etc) of a body. Also, the influence of various construction parameters or other design data on the main characteristics of the modes of motion is studied. The complex consists of two parts: lectures for a special course and computer support for it, given in the form of a library of programs for the calculation of the trajectories of motion and their visualization. In the lectures the simpler problems in the motion of a body in resisting medium, which admit analytical and qualitative research, are formulated and discussed. The computer support for the lectures can be used both by the professor and by students for studying more difficult problems, such as oscillations of an aerodynamic pendulum (weathercock), self-oscillations of the elastically fixed plate in a flow of medium (flutter), flight of a spinning finned shell (problem of external ballistics). The demonstrations of different parts of a complex on the computer is given. This is a joint work with Boris Lokshin and Yuri Okunev.

SHCHEPIN, Nick N (Donetsk Institute of Applied Math and Mechanics, Donetsk, Ukraine)

Modeling of elongated elastic body motion in liquid flow

The problem of a stationary flow of a viscous liquid around elastic rod was considered. The basic purpose of the work consisted in verifying the basic assumptions and laws, used at construction of models for motion of elastic rods in resistant medium. The elongated elastic bodies with variable bending rigidity and rather smoothly varied cross section were examined as the models of rod. Various types of rod's joints and initial forms of an axis were investigated. The relations for determination of parameters in dependences of forces and moment, acting on a rod on flow speed and geometry of the system were obtained. Configurations of the system for stationary flow were found.

STOROZHEV, Valery I (Donetsk State University, Ukraine)

Dynamic problems of the boundary layer theory for low-symmetric essentially anisotropic bodies, contacted with viscous liquid

New results of the investigations of the spectrum of three-dimensional normal waves in anisotropic plates of orthorombic class surrounded by viscous liquid with a significant quantitative difference in mechanical properties in various elastic-equivalent directions are presented. The effects of the influence of elastic materials' anisotropy and liquid medium's viscosity on the effects of the localization of wave movements in the border layer of solid bodies and liquid medium under various propagation directions are considered in detail. The possibilities of significant boundary layers with the intensity of localized waves' occurrence are investigated. The effects of leaky waves' energetical properties near the border of a solid body with liquid's contact are analyzed. The analogous results are obtained for cylindrical bodies having cylindrical orthotropy.

SUDAKOV, Sergey Nikitovich (Institute for Applied Mathematics and Mechanics, Donetsk, Ukraine)

Autorotation of a specific form plate, free-falling in the air

The autorotation of a specific form plate, free-falling in the air, is considered. The plate have the specific form and the specific mass distribution, like the form and the mass distribution of seed of mapl. For the plate of preassigned form two following problems are considered. (1) It is necessary to solve the problem of the existence of permanent autorotations for the plate with the preassigned mass distribution. (2) Let a part of parameters of the permanent autorotation is given. It is necessary to learn the distribution of mass for which such motion there exists.

VATULYAN, Alexander O (Rostov State University, Russia)

Boundary integral equations in research of the elastic bodies vibrations

Present article examines boundary integral equations arising in anisotropic theory of elasticity. The solution is found taking account of the a priori information about differentiability of the desired functions. Similar to the cubic splines approximation of the unknown functions has been created at the boundary of the domain.

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BROOK, Bindi S (University of Sheffield, UK)

A model for time-dependent flow in the (Giraffe) jugular vein

We present a computational model of blood flow in the (giraffe) jugular vein, based on the one-dimensional equations for flow in collapsible tubes. We investigate (a) the nature of the unsteady flow that results when the inflow rate is too large for steady flow to be possible (as predicted by Pedley, Brook and Seymour, Phil Trans R Soc Lond B, 351:855-866,1996), and (b) the way the flow adjusts during postural changes (e.g. head-down to head-up). In (a) small-amplitude oscillations arise; in (b) waves propagate up and down the vein, settling down to a steady state only after a time of up to 10 seconds.

This is a joint work with Timothy J Pedley, Cambridge University, UK.

DANIELSEN, Michael (Department of Mathematics and Physics, Roskilde University, Denmark)

The impact of ejection on ventricular performance

Ventricular performance is studied by coupling a model of the isovolumic ventricle to a description of the vasculature. This approach allows separation of ventricular and vasculature properties. The Frank mechanism and an ejection effect succeed in predicting ventricular performance during ejection. The ejection effect consists of two phenomena, pressure deactivation and hyperactivation, related to the detachment of crossbridge bonds and the formation of new bonds, respectively, during blood ejection. This may induce shifting of energy down the time axis.

This is a joint work with J T Ottesen, Roskilde University, Denmark, J L Palladino, Trinity College, Hartford, USA, A Noordergraaf, University of Pennsylvania, USA.

OLUFSEN, Mette (Center for Biodynamics, Department of Mathematics, Boston University, USA)

Arterial modelling: From data to real time simulation

We present a one-dimensional model of the systemic arteries which is validated against flow data from magnetic resonance measurements. The data represent flows averaged over the cross-sectional area in a number of vessels. The computed pressure profiles are used for validation of a simpler real-time lumped model which is part of a human patient simulator. The detailed model serves as a link between measured data and real-time simulations and can be used to investigate changes in arterial pulse due to changes in the vascular system.

This is joint work with Erik Morre Pedersen, Aarhus University Hospital and Jesper Larsen, Math-Tech.

THORUP, Pernille (Math-Tech, Copenhagen, Denmark and Technical University of Denmark, Lyngby, Denmark)

Vortex motion in the left ventricle

We present the flow fields from both a 2D and a 3D computational model of the left ventricle of the human heart. The models are developed by C Peskin and D McQueen using the Immersed Boundary Method. The computational results are compared to 3 directional magnetic resonance (MR) measurements of the flow field in the human heart. Special emphasis is placed on the vortex formation in the left ventricle, where both a qualitative and a quantitative comparison is carried out.

This is joint work with Charles Peskin and David McQueen, Courant Institute of Mathematical Sciences, New York University, USA.

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BANASIK, John L (University of Edinburgh, UK)

Regression and Arima models

A regression model predicts values of a dependent variable using an appropriate weighting of various explanatory variables plus a random error variable. These variables can include lagged values of the dependent variable to include aspects of delayed adjustment and lagged values of the error variable as a proxy for omitted variables. A multi-equation model can distinguish between direct and indirect influences of explanatory variables. An ARIMA model may be roughly described as a regression model that excludes genuine explanatory variables but which includes lagged dependent variables and/or lagged error variables each with potentially several different lags.

DOUTRIAUX, Jerome A (Faculty of Administration, University of Ottawa, Ottawa, Canada)

Qualitative and long term forecasting

Technology or long term forecasts are a combination of discontinuities and breakthrough with extrapolations of current trends and relationships. Whereas trends and relationships can often be modeled with time series or diffusion/substitution models if historical data is available, discontinuities and breakthrough must generally rely on the advice of experts. Some of the diffusion/substitution models currently used by high-technology enterprises will be presented, as well as the pseudo-quantitative methods developed to assess the internal consistency of qualitative expert forecasts; examples of application will be provided.

NASH, John C (Faculty of Administration, University of Ottawa, Canada)

Forecasting: A framework and graphical approaches

Forecasting takes place in the context of human activity and interests. Therefore the framework of any forecasting effort comprises assumptions of scale and environment as well as data and methods. An attempt will be made to present this framework for a number of examples. Many forecasting problems can be resolved by methods that are at some level very simple. Graphical techniques lend themselves extremely well to a large number of conventional administrative and business forecasting situations, and some examples of these will be presented.

CHENEY, Margaret (Rensselaer Polytechnic Institute, USA)

Acoustic and electromagnetic distinguishability in the half-space geometry

We consider the question of what measurements contain the most information about an unknown lower half-space. We translate this question into the mathematical problem of maximizing the ratio of the total upgoing energy to the total downgoing energy. The downgoing wave that maximizes this quotient is the best incident field to use.

Similarly, we can determine the measurements that are best for distinguishing an unknown lower half-space from a known (guessed) one. To do this, one should solve a similar maximization problem in which the total upgoing energy is replaced by the difference between the total upgoing energy (measured) for the half-space that is unknown and the total upgoing energy (calculated) for the half-space that is known. In the case of a medium that varies only in the vertical direction, the maximization can be carried out explicitly. In the case of an unknown medium, this maximization can be found by an iterative process.

CHERKAEVA, Elena (University of Utah, USA)

Inverse homogenization and the recovery of microstructural information in composite media

The talk deals with inverse homogenization problem for a medium with a microstructure, such as sea ice or a composite material. The problem is to find microstructural parameters from known response of the medium to applied electromagnetic field. When the wavelength of the electromagnetic field is much larger than the microstructural scale, fine scale variations in the complex permittivity cannot be resolved, and the microstructure on the fine scale is averaged out, or homogenized. However, it is still possible to deduce some information about the microstructural parameters of the medium, such as geometry or the volume fractions of the constituents, from averaged electromagnetic measurements. By exploiting an analytic representation of the effective complex permittivity, we reduce the problem of inverse homogenization to the problem of reconstruction of a spectral measure containing information about the geometrical structure of the material. Uniqueness of such reconstruction is discussed and shown that the problem is extremely ill-posed. To ensure stability of numerical solution, different regularization methods are introduced in computational scheme. As an example, we use this approach for estimating the thermal and fluid transport properties of sea ice using measurements of the complex permittivity of the sea ice mixture.

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WINEBRENNER, Dale P (University of Washington, USA)

Inversion of the 1-D Helmholtz equation: Application to the physical world

The achievement of stability in the presence of noise afforded by causally-stabilized layer-stripping overcomes one of the most fundamental obstacles to application of 1-D inverse theory to explore the physical and geophysical world. The rigorous formulation of such layer-stripping, however, presumes the availability of infinite-bandwidth information i.e., that the reflection response of a 1-dimensional medium is characterized at all frequencies from zero to infinity. Available information in any physical application is limited, so it is of interest to quantify the effects of limited bandwidth on the fidelity of reconstructions. The close parallels between linear Fourier transform theory and causally-stabilized layer stripping provide a natural framework for such a quantification. In this talk, I outline the derivation of such a quantification and discuss how the resulting insight can be derived in the sounding of terrestrial and extraterrestrial ice sheets and other applications.

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BORODICH, Feodor M (Department of Mathematics, Glasgow Caledonian University, UK)

Self-similar models and size effect of multiple fracture

Multiple fracture of polyphase quasi-brittle materials is analysed from the standpoint of similarity methods. First, two self-similar models of development of a cloud of micro- and meso-cracks in an unbounded solid are constructed. Both presented models supposed that the main part of the process zone is wedge-shaped and the process zone is bounded by an arc of a circle with the center at the main crack tip. The former model is based on the hypothesis of discontinuous self-similar character of the main crack propagation, while the latter model employs physical fractal approach. Finally, the problem of size effect for bounded models is studied. It is assumed that the main cause of the size effect is that the process zone cannot be fully developed in a bounded model of a real size construction.

GOMATAM, Jagan (Glasgow Caledonian University, UK)

Fractal morphology of deposits in heat exchangers and their physical properties

Our fundamental hypothesis here is that aggregates of deposits on a substrate inside a heat exchanger can be construed as media endowed with fractal properties over a finite range of temporal and spatial scales. We present image analysis of industrial deposits that confirm their fractal morphology; we then derive an equation governing the fouling resistance which displays an explicit dependence on the Sierpinsky fractal dimension. Extension of these ideas to aggregates on high temperature filters and their effect on filter efficiency will be outlined. This is a joint work with Dr Anthony J Mulholland, and was funded by E U in partnership with National Engineering Laboratory.

LOUIS, Enrique (Universidad de Alicante, Spain)

Scaling laws in fracture

The experimental and theoretical work carried out to identify scaling laws in fracture is reviewed. The benefits and drawbacks of the search for scaling and eventual fractality of cracks in brittle materials are discussed. In particular, we discuss the use of spring models to simulate crack propagation in brittle materials. A correspondence between the equations of motion and those of continuum elasticity can be made. The numerical scheme can be applied to analyze problems such that of quasistatic fracture, fracture induced by a thermal gradient or dynamic fracture. Recent work carried out to investigate the dynamics of cracks in brittle material when the velocity of the crack is comparable to the sound velocity, is discussed in some detail. Inertial and damped dynamics are analyzed. It is shown that dissipation strongly influences the shape of the crack. While inertial cracks are highly unstable, dissipation stabilizes straight cracks. The results can help to explain recent experiments on PMMA.

This is a joint work with F Guinea, Instituto de Ciencia de Materiales, Consejo Superior de Investigaciones Cientificas, Cantoblanco, Madrid, Spain and L M Sander, Physics Department, The University of Michigan, Ann Arbor, USA

ONISHCHENKO, Dmitry A (Institute for Problems in Mechanics, RAS, Moscow, Russia)

Strength of fractal trees and renormalization group method

A fractal tree (FT) is a hierarchical branching structure whose elements have random strengths. It is used in probabilistic failure/strength modelling for systems with localized load redistribution under progressive failure. The c.d.f. P_k of the strength of a k -level FT is given by recursive equations (REq): $P_i(x) = 2P_{i-1}(x)P_{i-1}(g(x)) - P_{i-1}^2(x)$, $i = \overline{1, k}$, where the load function g is non-decreasing and $g(x) \geq x$. With the notation $P_k = \mathcal{F}\{k, P_0\}$, the intrinsic group property leads to the Lie differential equations (DEq) $\mathcal{F}'_i(t, P_0) = \beta(\mathcal{F})$, $\beta(P_0) = \mathcal{F}'_i(0, P_0)$, where t is a real variable rather than integer. Using the renormalization group method, it is shown in the paper that the solutions of REq and those of DEq display a similar universal asymptotic behaviour under reasonable restrictions on P_0 .

SORNETTE, Didier (IGPP, UCLA, USA and CNRS, LPMC, France)

Failure prediction in heterogeneous materials using complex fractal dimensions

This research applies to composites, rocks, concrete under compression and materials with large distributed residual stresses. We find that rupture processes can be abrupt or critical depending on the amount of heterogeneity. For heterogeneous systems that fail by exhibiting a critical behavior, we introduce the concept of discrete scale invariance and its associated complex exponents and log-periodic signatures. The main idea is the combination of the concept of scaling together with the identification of a hierarchy of specific characteristic scales. This theory predicts precise signatures preceding failure, which have been tested extensively on gas pressure tanks embarked on the European Ariane rockets. We provide an introduction to the underlying theory, the physical mechanisms, as well as to generalization to other systems.

ALEXANDROV, Natalia M (NASA Langley Research Center, USA)

Using variable-fidelity models in multidisciplinary design optimization

We present an approximation management framework (AMF) for solving multidisciplinary design optimization problems with disciplines represented by computationally expensive models. AMF is based on a class of multilevel algorithms for large-scale nonlinear programming and it is aimed at maximizing the use of lower-fidelity, cheaper surrogate models in design problems. The talk will address theoretical and computational attributes of AMF, illustrated with numerical data.



LEWIS, Robert M (Institute for Computer Applications in Science and Engineering, USA)

A posteriori error analysis in nonlinear programming problems governed by differential equations

New techniques in a posteriori finite element error analysis enable the computation of quantitative bounds on the error due to discretization in functionals of the solutions of partial differential equations. We discuss incorporating these bounds in optimization using inexact function and gradient information, both for derivative-free (pattern search) and gradient-based (quasi-Newton) algorithms. The quantitative error bars from the bound procedure and the requirements of the optimization algorithms guide adaptive mesh refinement to determine acceptable steps. This has the effect of reducing the computational cost associated with unnecessarily fine meshes.

PATERA, Anthony T (MIT, USA)

Bound approximations for outputs of partial differential equations

We describe a Neumann-subproblem a posteriori finite element procedure that provides inexpensive, rigorous, sharp, and quantitative ("constant-free") lower and upper asymptotic bounds for linear or nonlinear functionals of the solutions to partial differential equations (e.g., moments, heat transfer rates, amplitudes, frequencies, lifts, or flowrates). Examples are drawn from symmetric and nonsymmetric coercive linear problems (elasticity, convection-diffusion), noncoercive linear problems (the Helmholtz equation), constrained problems (the Stokes system), nonlinear equations (eigenvalue problems, incompressible Navier-Stokes), and parabolic problems (the heat equation). Emphasis is placed on the application of these methods within the context of engineering design and optimization. This is a joint work with L Machiels, J Peraire, Y Maday.

SCHEINBERG, Katya (IBM, T J Watson Research Center, USA)

Extensions of DFO algorithm to constrained optimization

We consider a class of nonlinear optimization problems with "expensive" objective function and constraints. For such problems the derivatives of the objective function and, possibly, constraints are considered unavailable. Also some noise may be present in the function computations. This framework makes most of the "standard" nonlinear optimization techniques useless. Recently a class of, so called, derivative free optimization (DFO) algorithms was developed for unconstrained problems. The convergence theory and numerical results were reported. The method is based on using polynomial interpolation of the objective function in a trust-region framework. In this talk we consider extension of DFO methods to the case when constraints are present. Different type of constraints are considered: those whose function values are expensive to compute and those whose function values are cheap and whose derivatives are available. We discuss convergence theory and present computational results.

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HINDER, Rainer (Weierstrass-Institut fuer Angewandte Analysis und Stochastik im Forschungsbund Berlin e.V., Germany)

Analysis and numerics of the conical diffraction problem

In this talk we consider the diffraction of a time-harmonic oblique incident plane wave by a periodic optical grating which is invariant in one direction. Starting from the Maxwell equations one obtains two scalar Helmholtz equations which are coupled via transmission conditions on the interfaces of the grating and where the solutions have to fulfil nonlocal boundary conditions on some artificial boundaries. Based on a strongly elliptic variational formulation of the problem in a bounded periodic cell we present some existence-, uniqueness and regularity results and some numerical calculations.

KONDRAT'EV, Vladimir A (Moscow State University, Russia)

On evolutionary equations in nonsmooth domains

We study solutions of evolutionary equations in $\Omega \times [0, T]$, where $\Omega \in \mathbb{C}^n$ is piecewise domain. We consider the hyperbolic systems, the parabolic system, the Schrödinger equation and some nonlinear problems. The class of operators considered includes second order hyperbolic equations with mixed Dirichlet-Neumann conditions, the dynamic elasticity systems and others. Intersections and union of simple geometrical objects such as cylinders, cones, balls, or half-spaces usually have edges and corners that give rise to singularities of solutions in such bodies. The precise description of these singularities can be used for the construction of effective numerical approximation methods.

Let $L = \frac{\partial^2}{\partial t^2} - \sum_{|\alpha| \leq 2m} D^\alpha a_\alpha(x, t) D^\beta$ be an hyperbolic operator in $\bar{\Omega} \times [0, T]$, where Ω is a bounded Lipschitz domain. We shall describe the structure of weak of solutions $Lu = f$ near singularity points of $\partial\Omega \times [0, T]$.

KRUTITSKII, Pavel (Moscow State University, Russia)

Helmholtz equation in cracked domains

Dirichlet and Neumann problems for the dissipative Helmholtz equation in a plane domains bounded by closed and open curves are studied. Open curves model cracks in physical and mechanical applications. With the help of potential theory, the problems are reduced to the uniquely solvable integral equations at the boundary. Existence and uniqueness theorems are proved. The solution can be computed by standard codes by means of discretization and inversion of a matrix. Results for propagative Helmholtz equation in exterior domains are also formulated. See: P.Krutitskii, [1] *Applicable Analysis*, 62(1996), 297-309, [2] *Zeitschr. Analysis u. Anwend*, 16(1997), 349-361, [3] *ZAMM*, 77 (1997), 883-890.

LASIECKA, Irena (University of Virginia, Charlottesville, USA)

Wellposedness and asymptotic behaviour in nonlinear dynamic elasticity

The main aim of this talk is to present several results pertaining to uniform stability in models of nonlinear dynamic elasticity accounting for thermal effects. These models are described by elastodynamic 2-d system coupled nonlinearly with the Kirchoff plate and two heat equations. Depending on the model considered one may have or nonlinear coupling between the thermal and elastic equations. Both cases will be considered. The boundary conditions associated with the model are: free, for the mechanical displacements, and Robin's for the thermal variables. As usual, in the case of free boundary conditions, the boundary conditions are strongly and nonlinearly coupled.

The main results presented describe: (1). Wellposedness of the solutions for the overall nonlinear system. This includes existence and uniqueness of finite energy solutions, as well as their regularity for the initial data displaying more regularity. (2). Uniform decay rates (in time variable) for weak solutions.

LIFANOV, Ivan K (Airforce Engineering Academy, Russia)

Singular solutions of singular integral equations and their applications

A great attention has been recently paid in aerodynamics to the investigation of wing with the energy high-lift devices which includes external flow suction as a constituent part. The determination of the aerodynamic characteristics of the wing with the subsonic flow of ideal non-compressible fluid around reduces to a determination of the density of the vorticity layer by which it is simulated. It is shown that this problem reduces to solving a singular integral equation of the first kind on a curve in the class of functions which has at the suction point the Cauchy principal value integrable singularity. These solutions to singular integral equations are called singular solutions. Similar situation we have when we solve the problem of removing luminescence of contour angle points by location of current sources on a counter near these points in the antenna-diffraction problem. For the characteristic singular integral equations of the first kind on a segment the mathematical method of computation for such solutions is given.

MATVEEV, Alexander F (State Science Center of Russian Federation, ITEP, Russia)

Singular integral equations with negative index: Theory, approximate solutions and applications in aerodynamics

Boundary-value problem for Laplace equation that simulates flow around profile reduces to a complete singular integral equation (SIE). Solving these equation, if Hadamard correctness conditions are violated we have to use methods of regularization. The known scheme of regularization is suitable for characteristic SIE and not always good for complete SIE. Our paper presents examples of equations, for which known methods of regularization give extraneous solutions and introduces method of complete SIE regularization that does not demand additional restrictions. Using this method we construct and prove calculating schemes for complete SIE and present results for concrete aerodynamic problems.

MEDKOVA, Dagmar (Mathematical Institute, Academy of Sciences of the Czech Republic, Czech Republic)

Construction of the solution of the Dirichlet problem in nonsmooth domains

Boundary-value problem for Laplace equation that simulates flow around profile reduces to a complete singular integral equation (SIE). Solving these equation, if Hadamard correctness conditions are violated we have to use methods of regularization. The known scheme of regularization is suitable for characteristic SIE and not always good for complete SIE. Our paper presents examples of equations, for which known methods of regularization give extraneous solutions and introduces method of complete SIE regularization that does not demand additional restrictions. Using this method we construct and prove calculating schemes for complete SIE and present results for concrete aerodynamic problems

NISHIMURA, Naoshi (Department of Global Environment Engineering, Kyoto University, Japan)

A Galerkin fast multipole boundary integral equation method for elastostatic crack problems in 3D

The proposed paper discusses a fast numerical method of solving large scale elastostatic crack problems in 3D based on the Galerkin fast multipole boundary integral equation method. The proposed formulation uses the multipole expansion of the elastostatic double layer potentials in terms of 4 types of moments. This formulation is applied with Galerkin's method to the variational equation derived from the hypersingular integral equation for crack problems. It is confirmed through numerical experiments that the proposed method solves large problems involving hundreds of cracks accurately.

TAIRA, Kazuaki (Institute of Mathematics, University of Tsukuba, Tsukuba, Japan)

Diffusions and boundary value problems

My talk is devoted to the functional analytic approach to the problem of construction of Markov processes with boundary conditions in probability theory. We construct a Feller semigroup corresponding to such a diffusion phenomenon that a Markovian particle moves both by jumps and continuously in the state space until it dies at the time when it reaches the set where the particle is definitely absorbed.

TRENOGIN, Vladilen A (Moscow State Steel and Alloys Institute, Russia)

Generalized Lagrange formula and abstract boundary value problem

The system of two linear operator equations is considered. Every equation in the own Banach space is defined. The concepts of dual in Lagrange sense operator, Lagrange bilinear functional and generalized Lagrange formula are introduced. This approach permits to investigate some nonlocal boundary value problems for DE in composite domains including nonlinear problems with parameters and bifurcation of its solutions.

UMEZU, Kenichiro (Maebashi Institute of Technology, Japan)

Elliptic problems with nonlinear boundary conditions

This talk is devoted to the study of a class of semilinear elliptic boundary value problems with nonlinear boundary conditions. The continuation method or the implicit function theorem is used to prove the existence of smooth branches of positive solutions. The characterization of the branches, and the uniqueness and asymptotic behavior of positive solutions are studied by using some comparison principles with semilinear elliptic boundary value problems with linear boundary conditions.

ZHAO, Jennifer (University of Michigan-Dearborn, USA)

A nonlinear parabolic equation modeling surfactant diffusion

In this work, we will study a nonlinear parabolic system of equations in one dimensional space which models surfactant diffusion. We will study the well-posedness of the problem, and prove the uniqueness and existence of a solution to the problem.

BAKER, Christopher T H (Manchester University, UK)

Numerical treatment of retarded differential equations: Smoothness, stability, convergence, and practical design problems

Real-life phenomena often incorporate memory and time lag and give rise to retarded functional differential equations. These are characterized by interesting dynamics, smoothness complications, and the need to record the history. The numerical analyst must be aware of modelling considerations and underlying theory, and address the issues of smoothness, stability, and convergence, as well as the practical design problems. We present some of the relevant mathematics.

BUCKWAR, Evelyn (Free University Berlin, Germany & University of Manchester, UK)

Numerical methods for retarded stochastic equations

Numerical analysts have in recent times extended their attention from the treatment of deterministic ordinary differential equations to the treatment of (i) stochastic differential equations, and (ii) deterministic delay differential equations. We address the principal issues involved in progressing to the numerical treatment of stochastic delay differential equations, a class of problems of practical interest and for which there already exist some *theoretical* results. This is a joint work with Christopher Baker, at Manchester.

FORD, Neville J (University College Chester, UK)

Numerical treatment of Volterra integro-differential equations: Qualitative behaviour and stability theory

Volterra integro-differential equations are used to model many phenomena across the physical and biological sciences. In many of the application areas the equations are characterised by nonlinearity in the integral and long time intervals. In this talk we focus on the question of how reliably numerical solutions to such problems reproduce the qualitative and stability behaviour of the true solution. We review existing results and focus on our recent work which applies Lyapunov-type stability analysis to the discrete equations.

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MSP-036
MSP-072

HU, Guang-Da (Harbin Institute of Technology, Japan)

Delays in modelling of controls

DDEs and NDDEs often occur in the engineering of automatic control. Some systems have unavoidable time delay in the signal flow between components. The delay usually results from the physical separation of the components and typically occurs as a delay between a change in the manipulated variable and its effect on the plant or as a delay in the measurement of the output. Sometimes the delay results from other effects, for example, friction of mechanical system. In the talk, DDEs and NDDEs in control engineering are illustrated by a temperature control system, a control system of metal rolling and a manipulator robot control system.

PAUL, Christopher A H (Manchester University, UK)

Numerical modelling of delays in economics

Economic modelling, by its very nature of simulating real-life systems, involves delays. These delays can arise in a variety of ways and, depending on their precise nature, can give rise to delay (DDEs), neutral delay (NDDEs), Volterra integro- (VIDEs) and Volterra delay integro- differential equations (VDIDEs), or more general functional differential equations. In this talk, I examine the Solow vintage capital growth model which is represented by a system of VDIDEs: For computational reasons, it is desirable to transform the model equations into a system of DDEs. The resulting system can be solved using the code Archi, and its solution displays some interesting dynamical behaviour.

RIHAN, Fathalla A (Helwan University, Egypt & Manchester University, UK)

Sensitivity analysis of parameters in modelling with delay-differential equations

Many problems in biomathematics for which observations are given in the literature can be modelled by a suitable delay differential equation, parameterized by an optimum vector p . Our aim is (i) to estimate the sensitivity of the state variables to the parameter p and (ii) to judge the sensitivity of the parameter p to the observations. The latter permits us to assess the change in parameter values due to noise in the data and to assess any nonlinearity effect.

SHAW, Simon (Brunel University, UK)

Optimal data stability estimates and numerical schemes for history integral formulations of linear viscoelastic problems

Optimal data stability estimates are presented for the solutions of quasistatic linear viscoelasticity problems written in Volterra form with fading memory. These allow a priori error bounds to be derived for semidiscrete finite element approximations to the solutions of these problems, as well as a posteriori error estimates for a fully discrete space-time finite element approximation. This is a joint work with John R. Whiteman.

SIMPSON, Charles (Chester College, UK)

Fractional integrals and derivatives

We review recent work on the solution of fractional differential equations and their numerical analogues. This builds on previous work by Lubich, Baker and Derakhshan in the 1980s and more recent work by (inter alia) Diethelm, Blank and Ford. We consider the practical application of numerical methods, and the relationship with the underlying analytical theory and properties of the equations. We conclude with some numerical examples.

TIAN, Hongjiong (Manchester University, UK)

Singular perturbations of delayed equations: Applications, theory & numerics

The equation $\epsilon y'_\epsilon(t) = ay_\epsilon(t) + by_\epsilon(t - \tau)$ represents a simple singular perturbation problem in delay differential equations. There are a number of realistic equations of a similar type in the literature. We ask what happens to $y_\epsilon(t)$ as $\epsilon \rightarrow 0$ and what happens to the corresponding numerical solution $\tilde{y}_\epsilon(t)$ defined by a standard formula as the discrete mesh is refined.

WULF, Volker (University College Chester, UK)

Bifurcation and its numerical approximation in delay equations

We consider the question whether discretisations of delay differential equations preserve qualitative features. We are going to present different approaches in the analysis of numerical methods applied to delay differential equations undergoing Hopf bifurcations. Each of them having merits and drawbacks.

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MSP-037

FOKAS, Athanasios S (Department of Mathematics, Imperial College, UK)

An integral transform method for the Laplace equation in an arbitrary polygon

Using the relation between the harmonic functions of two variables and the analytic functions of one complex variable as well as the An integral transform method for Lax representation for the two dimensional Laplace equation, we find a new representation for the function analytic in the interior of any polygon in terms of its boundary values. This can be treated as an extension of the classical Fourier analysis. The method allows us to solve mixed boundary problems for polygons and dock problems for the half-plane. This is a joint work with Dr Andrei A Kapaev.

PELLONI, Beatrice (Imperial College, Mathematics Dept., London UK)

Linear and integrable nonlinear PDEs in arbitrary domains

A new spectral method for solving initial boundary value problems for linear and integrable nonlinear PDE's in two independent variables was introduced in A S Fokas, *A unified transform method for solving linear and certain nonlinear PDE's*, Proc. Royal Soc. Series A, 453 (1997). A general methodology for implementing this method in the case of arbitrary domains is presented in A S Fokas, B Pelloni, *A spectral method for linear and integrable nonlinear PDE's in arbitrary domains*, preprint (1998). The nonlinear Schrödinger, the sine Gordon and the Korteweg-deVries equations, as well as the linearized version of these equations in the domain $\{x \geq l(t), 0 \leq t \leq T\}$ are used as illustrative examples of this methodology. It is shown that there exist two distinguished cases: (a) If $l''(t) < 0$, then the solution of the linear and of the nonlinear equations can be obtained through the solution of a scalar and of a matrix Riemann-Hilbert (RH) problem respectively; this RH problem is defined on a *time-dependent* contour. (b) If $l''(t) > 0$, then the RH problem is replaced by a d-bar problem, defined on a *time-independent* domain. The scalar RH and d-bar problems can be solved in closed form, while the solution of their matrix analogues can be reduced to the solution of a linear integral equation. For linear PDE's this method provides the constructive implementation and the generalization of the celebrated Ehrenpreis principle; in the nonlinear case, it provides the extension of this beautiful result to integrable nonlinear PDE's.

SUNG, Li-Yeng (University of South Carolina, USA)

Initial-boundary value problems for linear evolution equations on the half-line

In this talk we will discuss recent results for initial-boundary value problems on the half-line obtained by the inverse spectral method. Explicit representations of solutions will be presented, together with their applications to the study of long-time phenomena.

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MSP-040
MSP-041

AINSWORTH, Mark (Strathclyde University, Glasgow, UK)

A posteriori error estimation for singularly perturbed problems

The talk will discuss a posteriori error estimation for finite element approximations of singularly perturbed problems such as $-\Delta u + \kappa^2 u = f$ and the associated elliptic system $-\Delta u + \kappa^2 B u = f$. It is shown that the standard a posteriori error estimators are not robust in at least one of the limits $\kappa \rightarrow \infty$ or $h \rightarrow 0$, where h is the mesh-size of the discretisation. This means that the estimators are either overly pessimistic or unreliable. A technique is described that leads to a fully robust a posteriori error estimator that provides guaranteed upper bounds on the true error that do not degenerate in either limit.

BABUSKA, Ivo M (Texas Institute for Computational and Applied Mathematics, University of Texas at Austin, USA)

Guaranteed A-posteriori upper and lower bounds for the exact error in the FEM and their iterative enhancement

The reliability interval is defined as the difference between the upper and lower bounds for the error in the computed data of interest. The talk will present the basic theory and computational illustration for the determination of the reliability interval and how it can be computed to a given tolerance. This is joint work with T Strouboulis.

PERAIRE, Jaime (Dept. of Aeronautics and Astronautics, Massachusetts Institute of Technology, USA)

Adaptive bound computations for functional outputs of partial differential equations

We describe a Neumann-subproblem a-posteriori finite element procedure that provides inexpensive, rigorous, sharp, and quantitative ("constant-free") lower and upper asymptotic bounds for linear or nonlinear functional of the solutions to partial differential equations (e.g., moments, heat transfer rates, amplitudes, frequencies, lifts, or flowrates). Examples are drawn from symmetric and nonsymmetric coercive linear problems (elasticity, convection-diffusion), noncoercive linear problems (the Helmholtz equation), constrained problems (the Stokes system), nonlinear equations (eigenvalue problems, incompressible Navier-Stokes), and parabolic problems (the heat equation). Emphasis is placed on the application of these methods within the context of mesh adaptive solution methods. This is joint work with L Machiels, Y Maday, and A T Patera.

STEIN, Erwin (Institute for Structural and Numerical Mechanics, University of Hannover, Germany)

Hierarchical finite-element- and model-adaptivity for composites

Based on dual error estimators for local Neumann problems, coupled discretization- and model-adaptivity is presented for hierarchically nested mathematical models of thin-walled composite structures, especially reinforced concrete plates. Error estimation is based on Posterior Equilibrium Method (PEM), equivalent to Residual Error Estimation Methods (REM), but yielding isotropic or anisotropic error estimates and avoiding locking effects, especially within model expansions in disturbed subdomains from lower to higher order kinematics and material equations, i.e. yielding appropriate effectivity indices. Examples show the efficiency of the method which provides a quality jump of FEM. This is a joint work with Erwin Stein and Stephan Ohnimus.

STROUBOULIS, Theofanis (Dept. of Aerospace Engineering, Texas A&M University, USA)

A-posteriori estimation and adaptive control of the error in the quantity of interest in the FEM and GFEM

This work addresses the problem of the a-posteriori estimation for the classical FEM and Generalized FEM. By Generalized FEM we mean the method which augments the basis of the standard FEM by including special functions which are known to approximate well the exact solution, e.g. singular functions at the corner points, and harmonic functions which satisfy the boundary-condition on a curved boundary, etc. The construction of the a-posteriori estimates is based on the splitting of the error into local and pollution error and the constructions of estimates for each component separately. This is joint work with I Babuska.

WHITEMAN, John R (Brunel University, UK)

A posteriori error estimates for quasistatic linear viscoelasticity problems

A space-time finite element method is proposed for quasistatic linear viscoelastic problems, modelled using history integral constitutive equations. For this a posteriori error estimates are presented which can be employed in the construction of adaptive schemes for problems of this type.

WOHLMUTH, Barbara (University Augsburg, Germany)

Local A posteriori error estimators for nonconforming discretization techniques

Local a posteriori error estimators are introduced and analyzed for mortar finite element methods. The pointwise continuity condition at the interface is replaced by a weaker condition involving Lagrange multipliers. The resulting nonconforming method is still optimal for several choices of discrete Lagrange multiplier spaces. Both hierarchical and residual based error estimators are introduced and analyzed. The case of discontinuous coefficients, the influence of the choice of the Lagrange multiplier and the coupling of different discretizations techniques are considered. It is shown that an appropriate measure of the nonconformity of the mortar finite element solution is a weighted L^2 -norm of the jumps across the interfaces. Numerical results illustrates the performances of the error estimators.

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BARTON, Noel G (CSIRO Mathematical and Information Sciences, Australia)

Use of the discrete element method to simulate mineral ore grinding mills

Mineral ore grinding mills break chunks of rock into smaller pieces. They are capital-intensive and expensive to operate. Motions within the mill can be simulated using the Discrete Element Method, which involves tracking of collisions, trajectories and spins of rocks. Interactions between the charge and boundary segments are also modelled. Various particle shapes are investigated. Simulation leads to improved understanding, enabling greater throughput, less wear on components and better efficiency. Results of 2D and 3D computer simulations will be displayed. Predictions are made for important aspects such as power draw of the mill, wear on lifter bars and intensity of collisions.

CLEARY, Paul W (CSIRO Mathematical and Information Sciences, Australia)

Modelling heat and fluid flow in high pressure die casting using smoothed particle hydrodynamics

High pressure die casting (HPDC) is used extensively in automotive industries to fabricate complex components from aluminium and magnesium. Liquid metal is injected into the mould at high speeds. Smoothed particle hydrodynamics (SPH) is used to improve understanding of HPDC leading to reductions in reject rates for cast components. Two and three dimensional simulations of the filling of several dies are presented for Reynolds numbers from 50 to 50,000. They show complex flows with recirculations, vortices, back filling, droplet and fragment formation. Heat transfer effects include temperature dependent viscosity and latent heat release during solidification, viscous heating and surface radiation. Detailed comparisons with experiments demonstrate close agreement.

JUNK, Michael (ITWM Kaiserslautern, Germany)

High speed inflation with SPH

We consider a two dimensional model of a balloon which is inflated with a high speed gas flow. The balloon tissue is assumed to be inelastic. Pressure and bending forces determine the equations of motion for the tissue which turn out to be a differential algebraic system. For the compressible gas flow, which is described by Euler equations, the tissue appears as a moving rigid wall, giving rise to a complicated moving boundary. This setup suggests the use of SPH as solver for the gas evolution. A careful treatment of boundary conditions with SPH deserves special attention in this problem.

STEINER, Konrad (ITWM Kaiserslautern, Germany)

The use of LBE in filtration processes

In many industrial applications filters are used to separate fluids, i.e. oil from water or air. Filter materials are porous media and their micro-structure influence the effectiveness of the filtration. The Lattice-Boltzmann method is used to simulate the two-phase flow through small, representative parts of porous media. A geometrical model represents the micro-structure of porous media by a stochastic distribution of the basic material elements. Quantities like relative permeability or capillary pressure can be calculated to predict the behaviour of the filter material and give the model parameters for numerical calculations based on Darcy's law.

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KISHIMOTO, Kazuo (University of Tsukuba, Japan)

Spectral properties of the operators which appears in the GARCH(1, 1) model

By using a Perron-Frobenius type theorem for positive operators, explicitly given are the second and the third largest eigenvalues of the operator which appears in the analysis of GARCH(1, 1) model. This result is a special case of a more general theorem which characterizes the second and the third largest eigenvalues for a certain class of positive operators.

KUSUOKA, Shigeo (Graduate School of Mathematical Sciences, University of Tokyo, Japan)

Approximation of expectation on diffusion model in finance

We give a new method to compute the price of European Exotic Options numerically. Our method is based on SDE, Lie algebra and analytic estimates derived by Malliavin calculus.

SHIRAKAWA, Hiroshi (Tokyo Institute of Technology, Japan)

Financial derivative evaluation by a simple low discrepancy sequence

We propose a simple class of generalized faure sequence which can be used to the efficient high-dimensional numerical integration. The essential difference between the original faure sequence to our sequence is that, we modify the sequence depend on the dimension and permute their dimension. Through these operation, we can drastically decrease the discrepancy of the points, especially for the high dimensional uniform distribution case. Also we apply these result to the arbitrage free financial derivative evaluation and checked the computational efficiency through the various type of derivatives.

JACOBONI, Irene (University of Bologna, Italy)

Upgrading the performance of a neural network-based method to predict the secondary structure of proteins

It has recently been proven that Neural Networks are useful tools to predict secondary structure of proteins (see Rost and C Sander, *Combining evolutionary information and neural networks to predict protein secondary structure*, Proteins, 19, 55-72 (1994)). The performance of the network strongly depends on the amount of information used for the training. The first version of the predictor used, as training set, the few available protein crystallized at that time and the overall accuracy (measured by the ratio of well predicted amino acid over the total number of amino acids shown to the network) was around 60%. Now using the rapidly increasing number of crystals deposited in PDB, we could perform a new training with more than 600 non-homologous proteins. This procedure rose the accuracy of the predictor from 60% to 68%.

A further upgrading of the performance has been obtained inserting Evolutionary Information as input to the Network: briefly the input is not anymore the amino acid sequence of the protein, but a mathematical representation of the alignment of the protein with its homologous in Swiss-Prot. Going from single sequence to multiple sequence, rises the accuracy from 68% to 72%. The quality of the prediction, in terms of length of secondary structure segments, has been improved, once again, by a mathematical tool, namely a second network, that uses as input the output of the first. This second steps avoids situation in which, for example, a residue predicted in b-state is surrounded by residues predicted in the a-state. This procedure increases the overall accuracy from 72% to 74%. At this stage the accuracy of our method is comparable with the most efficient methods published so far (see D Frishman and P Argos, *Seventy-five percent accuracy in protein secondary structure prediction*, Proteins, 27, 329-335 (1997)). Further improvements will hopefully be provided by averaging the results over slightly different network to reduce random noise (a procedure called jury decision).

This is joint work with Carsten Peterson.

MAINO, Giuseppe (ENEA, Applied Physics Division, Bologna, Italy)

Algebraic and functional techniques for the structure and dynamics of macromolecules

I present some group-theoretical and functional analysis techniques, recently developed, that allow to solve in analytical form or provide a simple computational framework for a few problems relevant to both the structural and dynamical properties of molecules and proteins. Analogies with many-body classical and quantum problems in nuclei and atoms (superconductivity, metal clusters and giant resonances, etc.) are pointed out and a comparison between theoretical results and experimental data is performed.

MALLAMACE, Francesco (Dept. Nuclear Engineering, MIT, Cambridge, USA)

Relevant aspects of the use of the fractal geometry in the study of the structure of new complex materials, (Dendritic polymer systems and porphyrins)

Scaling concepts have been widely used to explore intra- and the inter-molecular structure of different complex fluid. In this work we show as the fractal geometry can be fruitful employed in the study of two different classes of new materials: dendritic polymer systems and porphyrins. Whereas porphyrins in water are characterized, depending on their concentration and the solution ionic strength, by the built-up of extended clusters, dendrimers or "starburst polymers" (a new class of regularly branched macromolecules with unique structural and topological features of large interest in science and technology) can display an internal self-similar structure.

Physics of both the systems have been studied recently by means of theoretical methods, MD simulation as well as experimental investigations, but although new insight has been gained, much remains to be done. We discuss how the combination of these techniques can give exact information on the fractal structure of porphyrins aggregates and on the nature of the related growth mechanisms. In addition we show that any aggregation kinetics have, on considering also MD simulation, an early stage driven by a reaction limited aggregation. Such a phenomenon seems to be universal in clustering processes.

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ENGL, Heinz W (Johannes Kepler Universitaet Linz, Austria)

Industrial Mathematics Curricula - Some Examples from Europe

In Germany, Helmut Neunzert introduced a Technomathematics curriculum that is highly succesful and has also influenced the Austrian Industrial Mathematics curriculum. We report about both and about the European Postgraduate program "Mathematics for Industry" within ECMI.

A central part of all these programs are modelling activities where students are directly involved with industry. We present some of these projects emphasizing the parts where students actually contributed.

MATTHEIJ, Robert M (Department of Mathematics, Technische Universiteit Eindhoven, Netherlands)

Computational engineering needs mathematicians

The advancement of science and technology has certainly been made possible to a large extent by the impressive achievements of computational science. Theoretical science and experimental science are not challenged but rather compelmended. In particular both the modelling and the development of new and faster methods (including their analysis and understanding) is a typically mathematical task. It is important therefore to have mathematicians who are fit to do this. Not only should this pay off in terms of development of methods and software for a particular engineering problem. Also the transferability is much better taken care of by mathematicians who are not exclusively linked to such a special engineering discipline. We shall give a few examples of our experiences in Europe, in particular at Eindhoven university.

PETZOLD, Linda (University of California, Santa Barbara, California, USA)

Starting a CSE graduate program: Observations and experiences

We relate our experiences in starting a CSE graduate program at University of California, Santa Barbara. Issues such as core curriculum, graduation requirements, broadening the CSE student experience, and undergraduate preparation will be discussed.

STRANG, Gilbert (Massachusetts Institute of Technology USA)

Open discussion on computational science and engineering

Classical numerical analysis has often been successful without a close connection to a specific scientific application. But the distance between algorithm and application is closing fast. The words "scientific computing" partly reflected the change. Now highly interdisciplinary academic programs in the new field of Computational Science and Engineering (CS&E) are growing quickly.

The speakers in this minisymposium will discuss "teaching" of CS&E. They will address questions such as (1) What common elements should programs have? (2) How can disciplinary barriers be overcome? (3) For what careers are we preparing students? (4) What topics can we teach (and should we teach)? The speakers will also describe their European and American experiences with specific programs, and engage members in the audience in discussing them.

SIAM plans a major conference in October 2000 on Computational Science and Engineering. The ICIAM session will include an open discussion led by Gilbert Strang, Massachusetts Institute of Technology, SIAM President.

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DURÁN, Mario (Universidad Católica, Chile)

Study of instability in binary alloy solidification processes: Theory and numerical results

The instability in binary alloy solidification processes is a frequent and difficult problem, which appears in many industrial procedures. We tackle this physical situation by studing, theoretical and numerically, the bifurcation of the solutions of a stationary mathematical model. We deal with a system of nonlinear elliptic equations involving the thermodynamical variables of concentration, temperature, speed and pressure. These equations take into account the diffusive and transport phenomena, and consider nonhomogeneous materials, since the physical parameters depend on the unknowns of the problem. We discuss modelling, existence and uniqueness of solutions as well as show numerical results.

ORTEGA, Jaime H (Universidad del Bío-Bío, Departamento de Matemática, Concepción, Chile)
Generic simplicity of the eigenvalues for the Stokes system in two dimensional space

We analyze the multiplicity of the eigenvalues for the Stokes operator in a bounded domain of \mathbb{R}^2 with Dirichlet boundary conditions. We prove that, generically with respect to the domain, all the eigenvalues are simple. In other words, given a bounded domain of \mathbb{R}^2 , we prove the existence of arbitrarily small deformations of its boundary such that the spectrum of the Stokes operator in the deformed domain is simple. We prove that this can be achieved by means of deformation which leave invariant an arbitrarily large subset of the boundary. The proof combines Baire's lemma and shape differentiation. However, in contrast with the situation one encounters when dealing with scalar elliptic eigenvalue problems, the problem is reduced to a unique continuation question that may not be solved by means of Holmgren's Uniqueness Theorem. We show however that this unique continuation property holds generically with respect to the domain and that this suffices to prove the generic simplicity of the spectrum.

ORTEGA-TORRES, Elva (Doutora em Matemática Aplicada, Chile)

Magneto-micropolar fluid equations: An iterational method

We present a new proof of the existence and uniqueness of strong solutions for the equations of a Magneto-micropolar fluid. We use an iterational approach and we prove that the approximate solutions constructed by using this method converge to a strong solution of these equations. We also give the convergence rate bounds for this method.

PICASSO, Marco (Département de Mathématiques, Ecole Polytechnique Fédérale de Lausanne, Switzerland)

Numerical simulation of free surface flows applied to solidification processes

A numerical model to simulate complex, two and three-dimensional fluid flows with free surfaces is presented. The unknowns are the characteristic function of the region containing the liquid, the velocity and pressure fields in the liquid region. A splitting method is used for time discretization. At each time step, two transport equations are to be solved, plus a generalized Stokes problem. The two transport equations are solved by means of a forward characteristic method on a fixed grid made out of small rectangular cells. The generalized Stokes problem is solved using a finite element formulation on a fixed triangular mesh. Numerical results are compared for several test cases: the collapse of a dam with a facing obstacle; the filling of a disk with core; the filling of an S-shaped channel; the filling and solidification of a liquid metal during a casting process.

ROJAS-MEDAR, Marko A (Universidade Estadual de Campinas, Brazil)

On magneto-micropolar equations: Theory and numerical analysis

During the last decades engineers and physicist have made many efforts to investigate numerically some properties of the magneto-micropolar model. The equations in this model describe the motion of a fluid taking into account the velocity, the micro rotational velocity, the magnetic field and pressure. We devote our study to the existence and uniqueness of the solution of the model in exterior domains in \mathbb{R}^3 . We consider both the evolution and the steady state.

Finally, we discuss the computations.

BAO, Gang (University of Florida, USA)

Some mathematical issues in diffractive optics

In this talk, recent developments on the mathematical modeling of diffractive micro-optics will be reported. Particular attention will be paid to a variational approach. The speaker will present mathematical and computational results for the diffraction problem in linear, nonlinear, as well as chiral grating (periodic) structures. Results on the inverse diffraction problem and the optimal design problem will also be discussed.

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MSP-048
MSP-049

BENDALI, Abderrahmane (INSA, Toulouse, France)

Impedance boundary conditions incorporating the effect of a thin coating in electromagnetic scattering

We start the exposure with some numerical experiments demonstrating that a direct solving of the problem relative to the scattering of an electromagnetic wave by a thin dielectric coating as if it is thick may completely fail because of the numerical instabilities that then arise. We then recall some procedures, either heuristic or rigorous, usually used to derive generalized boundary conditions which incorporate the effect of the thin coating in an approximate way. We will then show how asymptotic analysis can be used not only to do this derivation in a direct and systematic way but also to easily give error bounds resulting from the approximation process. We end the exposure with some indications on the numerical solution of the problems involving these impedance boundary conditions.

BONNETIER, Eric (Ecole Polytechnique, France)

Optimal design of 2-D periodic diffractive structures

Consider the problem of designing a periodic interface between two different materials that gives rise to a specified far-field diffraction pattern for a given incoming plane wave. The time harmonic EM waves are assumed to be TM (transverse magnetic) polarized. The diffraction problem is modeled by a generalized Helmholtz equation with transparent boundary conditions. The optimization problem is not well-posed over the class of interfaces which are graphs of piecewise smooth functions. By considering highly oscillatory profiles, a relaxed formulation of the optimization problem is given in this work. The principal idea is based on homogenization theory. We characterize the set of admissible (generalized) designs for the relaxed problem and establish the existence of an optimal design.

COSTABEL, Martin (Université de Rennes, France)

Nonsmooth electromagnetic problems and standard finite elements

We consider the discretisation of time-harmonic Maxwell equations with perfect-conductor boundary conditions by H^1 -conforming finite elements. In order to avoid the infinite-dimensional eigenspace corresponding to frequency zero, one can regularize the weak formulation by adding a divergence term. On polyhedral domains, this gives a well-posed problem in H^1 , but if there is a non-convex corner, the finite element method approximates this wrong solution. In this talk, this phenomena is shown for L-shaped waveguides, and possibilities of avoiding it are discussed.

DOBSON, David C (Texas A&M University, USA)

Numerical modeling of photonic crystals

Photonic crystals are periodic structures fabricated from dielectric materials. Such structures can be designed to exhibit band gaps in the propagation of classical electromagnetic waves, and other interesting spectral behavior. An efficient method for band structure calculations in photonic crystals is presented. The method uses a finite element discretization, coupled with a preconditioned subspace iteration algorithm. The numerical performance of the method is examined, along with applications to optimal design.

JOLY, Patrick (INRIA, France)

Space-time mesh refinement for Maxwell's equations

Local grid refinement in space and local time-stepping constitute a very important feature in practice for FDTD computations (using Yee's scheme for instance) in electromagnetism. Usual interpolation procedures generally lead to long time instability under usual CFL conditions. We propose here a new approach that guarantees the conservation of a discrete energy. We identify a general abstract framework that enables our approach to be extended to various approximation procedures in space.

MCLAUGHLIN, Joyce (Rensselaer Polytechnic Institute, USA)

One way electromagnetic waveguide calculations

We exhibit an operating splitting technique for calculations of the outgoing wave in a range and depth dependent waveguide. The Dirichlet to Neumann (and variations of this) map and operator Riccati equations are used in the calculations.

MONK, Peter (University of Delaware, USA)

Numerical analysis of magnetic media

We discuss the discretization of the Maxwell system augmented by the Landau-Lifschitz-Gilbert equation. This non-linear system models magnetic materials particularly on the micro-magnetic scale. We derive a set of invariants for the system and present a numerical scheme that preserves these properties. We show that this scheme can produce good simulations of some model problems. This is joint work with O Vacus, Dassault, France.

NÉDÉLEC, Jean-Claude (Ecole Polytechnique, France)

Maxwell's equations in chiral media

We derive the Drude-Born-Fedorov constitutive relations, governing the propagation of electromagnetic waves in chiral media, from the standard constitutive relations for a homogeneous, isotropic medium by embedding in the medium a large number of regularly spaced, randomly oriented helical conductors, each modeled as a dipole.

PERUGIA, Ilaria (Dipartimento di Matematica, Università di Pavia, Italy)

A mixed formulation for magnetostatics: Theoretical and numerical aspects

Standard formulations for Magnetostatics strongly enforce the constitutive equation and one of Maxwell's equations, while weakly satisfying the other one. Due to the usually poorly identified material properties, it would be preferable to impose Maxwell's equations strongly, while approximating the constitutive law. In this way, the problem is written as the linearly constrained minimisation of a quadratic functional, where Maxwell's equations represent the constraints. A mixed formulation obtained by imposing Maxwell's equations with Lagrange multipliers will be presented, highlighting the connection with classical mixed methods for Magnetostatics, and discussing a finite element method for the discretization.

SANTOSA, Fadil (Institute for Mathematics and its Applications, University of Minnesota, Minneapolis, USA)

An optimal design problem arising in diffractive optics

We study an optimal design problem arising in diffractive optics. A novel feature of this work is that we incorporate manufacturing constraints, and manufacturing uncertainties. We formulate an optimization problem whose solution is robust against the 'noise' introduced by the manufacturing process. The main ideas of the work will be illustrated in numerical simulations.

SCHMIDT, Gunther (WIAS Berlin, Germany)

Direct and inverse conical diffraction problems

The diffraction of time-harmonic electromagnetic waves under oblique incidence by periodic structures can be modeled as a system of two Helmholtz equations coupled via transmission conditions at the material interfaces. In the talk existence and uniqueness results for its variational formulation are presented, leading, in particular, to the stability and convergence of finite element methods. Further we consider the problem of designing multilevel optical gratings in such a way that diffracted waves have a specified far-field pattern for a given incident plane wave. This problem is formulated as minimization problem for certain cost functionals involving Rayleigh amplitudes. We obtain analytic and efficiently computable formulas for the gradients of these functions with respect to the geometric parameters of the grating.

VALLI, Alberto (Department of Mathematics, University of Trento, Italy)

Domain decomposition methods for the time-harmonic Maxwell equations

A domain decomposition approach based on finite element discretization is proposed for the solution of the low-frequency time-harmonic Maxwell equations. Two cases are considered: a non-homogeneous and non-isotropic conductor, and a composite medium, conductor in one part and perfect insulator in the other. Edge finite elements are employed in the conductor, while the problem is reformulated by means of a scalar potential in the insulator, leading to an elliptic boundary value problem which is approximated via piecewise-polynomial finite elements. An iteration-by-subdomain procedure is proposed, and it is shown to converge at a rate independent of the mesh size. The preconditioner implicitly defined by the iteration procedure is therefore optimal.

This is a joint work with Ana Alonso.



BROKATE, Martin (Mathematisches Seminar, Universität Kiel, Germany)

Nonlinearly coupled rate independent evolutions

Rate independent evolutions, or hysteresis operators, often appear as part of a dynamical system described by differential equations. We discuss several such situations and present mathematical results. We focus on the interplay between regularity properties of the hysteresis operators and of the solutions to the overall system.

CROSS, Rod (Department of Economics, University of Strathclyde, Glasgow, UK)

Hysteresis in economic systems

This paper describes how the Preisach model, with its superposition of hysteresis play operators, can be applied to economic systems. At the micro level economic agents, because of fixed or sunk costs of adjustment, adjust discontinuously to changes in state variables and have different trigger points for adjustment. Illustrations of this analytical framework are provided. Simulation exercises are pursued using plausible parameter values. A programme is then constructed to yield hysteresis measures for economic time series, which are then used to test for the presence of hysteresis in steady state relationships.

This is a joint work with Dr Michael Grinfeld, Mathematics, and Dr Laura Piscitelli, Economics, University of Strathclyde, Glasgow, UK.

DESCH, Wolfgang (Universität Graz, Austria)

The stop operator and elastic contact problems

We consider a unilateral contact problem for a linearly elastic beam partially fixed at one end. The problem leads to a one-dimensional hyperbolic PDE with contact boundary conditions. The method of characteristics leads to a fixed point equation involving the stop operator known from the theory of elastoplasticity. Existence and uniqueness of solutions follows from Lipschitz continuity of the stop operator in $W^{1,1}$.

DUPUIS, Paul (Brown University, USA)

Formulation of the Skorokhod problem in communication, queueing, and economics

The Skorokhod Problem defines a mapping on path space that can be used in many different ways to study processes that are constrained to a fixed subset of some Euclidean space. In this talk we will describe, in the context of 2-3 examples, how one identifies that Skorokhod Problem that is appropriate for a given applied problem. If time permits, some of the main applications of the Skorokhod Problem (functional law of large numbers, diffusion approximation, large deviations, stability analysis, etc.) will be mentioned.

GÖCKE, Matthias (University of Münster, Faculty of Economics, Germany)

Types of economic hysteresis

Different concepts of hysteresis utilised in economics are compared. Adjustment costs generate "real" hysteresis, i.e. multibranch-nonlinearity, where temporary exogenous shocks lead to switches between different "branches" of an entire relationship. The shape of the hysteresis loop changes when an aggregation towards a macroeconomic relation is conducted over heterogeneous microeconomic elements. Hysteresis-relations are based on a local structural instability in the case of a branch-to-branch-transition. However, the persistence characteristics of first order difference (differential) equations with unit (zero) roots, which are based on a global indifference-instability, are in economics often incorrectly labelled as "hysteresis".

HULE, Richard (Institute of Economic Theory and Policy, University of Innsbruck, Austria)

Hysteresis operators in economic models

Although hysteresis effects are well known results of economic decisions (e.g. sunk costs in investment problems or habit effects in consumer demand) these features are not usually incorporated into general equilibrium models. It is therefore an open question if the standard results of such models are stable with respect to hysteresis. equilibrium models leads to new questions of their behaviour especially with respect to random and/or higher dimensional inputs. The paper tries to set up a framework for addressing both, the economic and the technical questions.

KUNZE, Markus (Mathematisches Institut, Koeln, Germany)

State-dependent sweeping processes

State-dependent sweeping processes, or their equivalent quasi-variational inequalities (where the constraint set depends on the solution itself), appear in a wide range of applications, e.g. in plasticity, if the yield surface changes its form depending on stress and strain. We discuss a sharp existence theorem and indicate applications.

POKROVSKII, Alexei (Institute for Nonlinear Science, Department of Physics, National University of Ireland, Cork, Ireland)

Properties of the stop nonlinearity and analysis of feedback systems

The stop-nonlinearity is an important example of a sweeping processes with various applications. This nonlinearity, arising in hysteresis theory, has a rich and unusual list of properties when treated as an operator in functional Banach spaces. I will discuss how these properties can be "utilized" in investigation of feedback control systems with hysteretic nonlinearities, with special emphasis on stability and controllability analysis.

RAMANAN, Kavita (Bell Laboratories, Lucent Technologies, USA)

On Lipschitz continuity of the Skorokhod map on polyhedral domains

The solution to the Skorokhod Problem defines a deterministic mapping, referred to as the Skorokhod Map, that takes unconstrained paths to paths that are confined to live within a given domain G in \mathbb{R}^n . Given a set of allowed constraint directions for each point of the boundary of G , the solution to the Skorokhod Problem defines the constrained version Z of a path X , where the constraining force acts along one of the given boundary directions using the "least effort" required to keep Z in G . The map that associates the constrained process Z to the unconstrained process X is referred to as the Skorokhod Map. We focus on the case when the domain G is a convex polyhedron, with a constant and possibly oblique constraint direction specified on each face of G , and with a corresponding cone of constraint directions at the intersection of faces. We present results on sufficient conditions for Lipschitz continuity of the Skorokhod Map (with respect to the sup norm on path space) and motivate our analysis by some illustrative examples. This is joint work with Paul Dupuis, Brown University.

VLADIMIROV, Alexander (Institute for Information Transmission Problems, Russia)

Averaging properties of Skorokhod operators

We study the dynamical behavior of polyhedral Skorokhod problems and sweeping processes with oblique reflection interpreted as hysteresis input-output operators W with short memory. Our main concern is the class of "slowly drifting" inputs $u(t, \alpha(\tau(t)))$, where u is T -periodical in t for all fixed α , and τ is a slow time. We find conditions ensuring that any output $x(t) = Wu(t)$ converges to a slowly drifting output $x(t, \beta(\tau(t)))$. The dependence of the averaged output $\beta(\tau)$ on the averaged input $\alpha(\tau)$ can be described by another (averaged) Skorokhod problem or sweeping process.

The same way as for the unique solvability of the Skorokhod problem and for the Lipschitz continuity of its map, the sufficient conditions are expressed in terms of various kinds of stability of a finite set of special matrices: oblique projections on the faces of the characteristic polyhedral set.

ANITESCU, Mihai (Argonne National Labs, USA)

Time-stepping methods for stiff multi-rigid-body dynamics with contact and friction

The field of multi-body dynamics simulation is expected to have a major impact on the design of complex mechanical systems. Finding realistic models for impact and friction is an important issue when dealing with such systems. Unfortunately, it is known since the late century that the acceleration setting of the differential algebraic equations involving friction does not always have a solution.

Recently, a new setting was developed for the constrained Newton equations in presence of contact friction in which accelerations and forces are replaced by velocities and impulses. For all configurations, the new model is proven to have a solution that can be found by Lemke's algorithm. The new framework, based on a linear complementarity problem, mixes together the resolution of the velocities with the Euler integration step and treats the contact and impact configurations in a unified manner.

In this presentation we discuss the possibility of adapting this approach to cases that exhibit significant stiffness and for which a simple Euler step is expected to perform poorly. Much attention is given to linear implicit solvers, for which the resolution of a nonlinear complementarity problem can be avoided.

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KUNZE, Markus (Mathematisches Institut, Universitaet Koeln, Cologne, Germany)

On the application of Conley index theory to non-smooth dynamical systems

The Conley index is a well-established tool in proving the occurrence of bifurcations in classical dynamical systems. We indicate how it generalizes to non-smooth dynamical systems, which take into account for frictional or impact effects in the model. The equation we are going to consider describes the motion of the wings of a bird.

SCHATZMAN, Michelle (CNRS and Université Claude-Bernard Lyon 1, France)

Moreau's rule and penalty approximation

The impact dynamics for a system with a finite number of degrees of freedom can be described by a system of highly nonlinear differential equations, which include an assumption on the constitutive law of the impact. A particular case, called Moreau's rule, is when the tangential component of the velocity along the set of constraints is transmitted, while the normal component is set to 0. When a penalty approximation is applied to the system of differential equations which describe impact, the outcome of the limiting process as the penalty coefficient tends to 0 depends on the rule which has been chosen for the approximation. We give examples of different penalizations, covering the discrete time and the continuous time cases, and we show when Moreau's rule is obtained in the limit, and when it is not obtained. The techniques use validated asymptotics and the amount of geometry which is necessary in this context, so as to work in generalized coordinates, but no more.

STEWART, David E (Department of Mathematics, University of Iowa, Iowa City, USA)

Mathematics of impact and friction problems

Recently there has been a great deal of work on computational aspects of rigid body dynamics with unilateral contact and Coulomb friction, including complementarity formulations and time-stepping methods. These new computational methods can also help develop the basic theory of rigid body dynamics when coupled with a suitable convergence theory. Convergence theory developed by the speaker will be described, along with the newer time-stepping methods to which it can be applied.

STIEGELMEYR, Andreas (Institute B for Mechanics, Technical University Munich, Germany)

Impacts with friction - Theory and practice

Various models for impacts with friction have been proposed, the most successful ones taking into consideration a compression and an expansion phase in normal and tangential direction. Impulses are stored during compression and released with frictional losses during expansion. Stick-slip and detachment phenomena during the impact can be considered by complementarity rules. A corresponding model for impacts with friction is presented and verified by measurements with an impact machine. In addition, some industry applications confirm the theory.

ROUGEMONT, Jacques (Theoretical physics, University of Geneva, Switzerland)

Dynamics of interfaces in the Ginzburg-Landau equation

We consider the real Ginzburg-Landau equation $\partial_t u = \Delta u + u(1 - u^2)$ in one and two dimensions. This equation has two trivial stable solutions: the constant functions ± 1 . We call interface the layer separating a region where $u \approx +1$ and a region where $u \approx -1$. This interface tends to invade the smallest of the two regions at a very low speed. We discuss the qualitative difference between the 1D case and the 2D case. In both case, by working in infinite volume, we are able to use these "slow-moving" solutions to construct orbits of the equation which never come close to one of the two above-mentioned equilibria.

RUBIN, Jonathan (Ohio State University, USA)

Existence and stability of phase-slip solutions to the nearly real cubic Ginzburg-Landau equation

Using geometric methods, we show the existence of a heteroclinic connection, namely a wave with a phase jump, between periodic end states for the real cubic Ginzburg-Landau equation under an imaginary perturbation. The stability of this solution is considered rigorously via Evans function calculations, including series expansions on a Riemann surface. When the perturbation is regular, these reveal a parameter regime where the wave is linearly stable and another regime where the wave is nonlinearly stable. When the perturbation is singular, the wave is shown to be unstable in a certain parameter regime. This is joint work with Todd Kapitula.

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MSP-053

SANDSTEDTE, Björn (Ohio State University, USA)

Bifurcations from fronts and pulses caused by the essential spectrum

In this talk, we consider bifurcations from fronts and pulses that arise as travelling waves in reaction-diffusion systems on the real line. Fronts and pulses destabilize, for instance, if one of their asymptotic rest states destabilizes in a Turing bifurcation. This instability is caused by the essential spectrum that crosses the imaginary axis. Without the presence of fronts or pulses, a Turing bifurcation near a homogeneous rest state creates a continuum of stationary spatially-periodic patterns of small amplitude that are parametrized by their wavelength. If a travelling pulse destabilizes in this fashion, we show that a continuum of modulated pulses is created. These modulated pulses resemble a superposition of the primary pulse with the aforementioned small Turing patterns; the resulting patterns are time periodic in an appropriate moving coordinate frame. If the primary pattern is a moving front, and the rest state ahead of the front destabilizes, then modulated fronts bifurcate. If, however, the rest state behind the front destabilizes, modulated fronts are not created. To prove these results, the parabolic equation is cast as an elliptic equation in the spatial variable and recent results on exponential dichotomies for elliptic systems are exploited. This is joint work with Arnd Scheel, FU Berlin.

SCHNEIDER, Guido (Mathematisches Institut, Universität Bayreuth, Germany)

Stability of modulating fronts and pulses

We consider pattern forming systems in infinite cylindrical domains. Examples are classical hydrodynamical stability problems, but also systems in nonlinear optics. Modulating front and pulse solutions consist of an front or pulse like envelope moving in the laboratory frame and modulating an underlying spatially and temporarily oscillating pattern. Here we address the stability question of such solutions. Depending on the continuous spectrum of the linearization exponential or polynomial decay rates can be obtained.

VAN HECKE, Martin (CATS/ Niels Bohr Institute, Denmark)

Coherent structures and spatiotemporal chaos in the complex Ginzburg-Landau equation

The complex Ginzburg-Landau equation models extended systems near a Hopf bifurcation. Depending on coefficients, an abundance of spatiotemporal chaotic states have been found. These states appear to be built up from local structures with well-defined propagation and interaction behavior. We relate a new local structure to a homoclinic orbit in a low dimensional dynamical system. These structures dominate in a number of chaotic states, and we explain some basic properties of these structures and states.

BIELAWSKI, Serge (Université des Sciences et Technologies de Lille, France)

Hydrodynamics in optics: Understanding spectral waves in laser experiments using a multiple scale analysis

A multimode laser with inhomogeneous broadening behaves as a chain of locally coupled oscillators, each associated with one lasing mode. Using a multiple scale analysis, we identify two types of parametric instabilities for the modulated laser. The primary instability is similar to the Faraday instability in hydrodynamics, and excites stationary waves inside the laser spectrum. Far from threshold, this wave destabilizes through a cascade of parametric instabilities. This is expected to occur in other systems with a decreasing dispersion curve. Finally, we show numerically that nonuniformities induce self-sustained Eckhaus instabilities, and leads to a particular type of spatiotemporal chaos.

CARR, Thomas W (Southern Methodist University, USA)

Global mixed mode chaos in nonlinear optics

Bi-instability, in contrast to bistability, is shown to generate unstable chaotic saddles prior to the onset of chaos. The theory and numerics are applied to a CO₂ laser model with modulated losses where unstable pairs of saddles coexist, form heteroclinic connections, and allow mixing between local chaotic attractors to produce global mixed-mode chaos.

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GAVRIELIDES, Athanasios (Air Force Research Laboratories, USA)

Instabilities of semiconductor laser systems: Theory and experiments

The various models of semiconductor lasers subject to external influences will be presented and examined for their similarities and their bifurcation structure. The main focus will be on the semiconductor laser in an external cavity, and the rich dynamics that are possible in delayed differential equation systems. The multiple fixed points and coexisting periodic attractors will be discussed and experimental results will be presented. Further it will be shown both experimentally and numerically that as the feedback strength in this system is progressively increased, the laser undergoes a cascade of bifurcations where each external cavity mode becomes unstable and is replaced by the next one of higher intensity. In the stable regions the laser is operating in the maximum intensity external cavity mode and in the unstable regions the laser exhibits chaos which evolves into the low frequency fluctuation regime (chaotic itinerancy). It will be demonstrated that these complex dynamics can be effectively controlled experimentally by a novel technique called dynamic targeting.

MANDEL, Paul (Universite Libre de Bruxelles, Belgium)

Multimode laser dynamics

Intracavity second harmonic generation offers an experimental realization of N globally coupled nearly identical nonlinear oscillators. This system is characterized by antiphased dynamics arising from a primary Hopf bifurcation that is always degenerate. We show via a normal form analysis that this dynamics can be described in terms of an eigenvectors basis. Each eigenvector describes one type of antiphased solution. A secondary Hopf bifurcation leads to quasiperiodic states which can still be expressed in terms of the same eigenvectors. These eigenvectors introduce a natural hierarchy of dynamical states. The two Hopf bifurcations can coincide.

ROY, Raj (Georgia Institute of Technology, USA)

Clocks, chaos and communication: Models and experiments on laser systems

A review of laser nonlinear dynamics will be presented. Lasers with small numbers of modes of the electromagnetic field as well as those with thousands of modes will be discussed. The different types of models used will be described and illustrated with specific examples. The question of using chaotic lasers for communication will be addressed, and recent experiments that demonstrate communication using chaotic waveforms will be reported.

ACEVES, Alejandro B (University of New Mexico, USA)

Pulse dynamics in nonlinear optical fibers with long and short period Bragg gratings

The extraordinary ability of the existing technology to engineer grating assisted dispersion profiles, added to the nonlinear effects in the fiber, provide novel optical elements with interesting potential applications. In this talk, we will discuss the dynamics of pulses in optical fibers having both long and short period Bragg gratings. Applications such as all optical switches, buffers, pulse compressors and novel fiber lasers will be presented along with state of the art experimental results.

GABITOV, Ildar R (Los Alamos National Laboratory, USA)

Four-wave mixing in soliton optical fiber links with dispersion management

Wavelength division multiplexing (WDM) is currently one of the most effective ways to increase the transmission capacity of optical lines. Four-wave mixing (FWM) is the major factor which limits the potential of the WDM approach. This limitation is due to the nonlinear interaction of neighboring frequency channels which leads, in particular, to the generation of Stokes and anti-Stokes sidebands, that play the role of an extra noise source and lead to signal deterioration. Dispersion management is a powerful technique of fiber optic telecommunication. There are strong evidences that dispersion management helps also to suppress the FWM and, hence, makes it possible to realize the true potential of WDM. We study mathematical model of systems based on the soliton signal format in the presence of a dispersion map. Based on this study, we propose a way to minimize FWM-imposed limitations on data streams by choosing an optimal dispersion map.

KAPITULA, Todd (University of New Mexico, USA)

Stability of bright solitary-wave solutions to perturbed nonlinear Schrödinger equations

The propagation of pulses in ideal nonlinear optical fibers without loss is governed by the nonlinear Schrödinger equation (NLS). When considering realistic fibers one must examine perturbed NLS equations, with the particular perturbation depending on the physical situation that is being modeled. Given that a wave persists, it is then important to determine its stability with respect to the perturbed NLS. A major difficulty in analyzing the stability of solitary waves upon adding dissipative terms is that eigenvalues may bifurcate out of the essential spectrum. Since the essential spectrum of the NLS is located on the imaginary axis, such eigenvalues may lead to an unstable wave. In fact, eigenvalues can pop out of the essential spectrum even if the unperturbed problem has no eigenvalue embedded in the essential spectrum. Here we present a technique which can be used to track these bifurcating eigenvalues. This technique is very general and should therefore be applicable to a larger class of problems than those presented here. This is joint work with Björn Sandstede.

KUTZ, J Nathan (Department of Applied Mathematics, University of Washington, USA)

Dynamics and bifurcations of a planar map modelling dispersion managed breathers

We study a non-autonomous ODE with piecewise-constant coefficients and its associated two-dimensional Poincaré mapping. The ODE models variations in amplitude and phase of a pulse propagating in a lossless optical fiber with periodically varying dispersion. We derive semi-explicit exact solutions and use them to locate fixed points, describe their bifurcations and stability, discuss the global structure of the Poincaré map, and consider various physically realizable perturbations to the pulse propagation. This is a joint work with P Holmes, Princeton University, USA.

TRILLO, Stefano (Fondazione ugo Bordoni, Italy)

Recent achievements in optical gap soliton theory

We overview recent progresses in theoretical understanding of optical gap solitons, i.e. low-velocity solitons propagating in nonlinear periodic media (gratings). First, a stability theory for gap solitons is developed in the framework of a generalized massive Thirring model with cubic nonlinearity. Second, it is found that two-color gap solitons can be sustained by quadratic nonlinearities (i.e., parametric mixing such as second-harmonic generation) in periodic structures exhibiting either a single or twin gaps. These entities present interesting peculiar features such as the dynamical formation of zero-velocity solitons in the lab frame.

TURITSYN, Sergei K (Division of Electrical Engineering and Computer Science, Aston University, Birmingham, UK)

Internet equation

I overview recent progress in high-speed, high-bit-rate optical data transmission that is the key element in the Internet development. Properties and solutions of the nonlinear model, basic for this fast developing field will be discussed.

WABNITZ, Stefan (University of Bourgogne, France)

Dynamics of soliton collisions in strongly dispersion managed fiber systems

Soliton collisions in wavelength-division multiplexed soliton transmissions may lead to severe pulse distortion and time jitter which undermines the system performance. In the case of dispersion managed systems, an optimal dispersion map should be designed in order to reduce and possibly suppress the effect of collisions. In this talk we will discuss how a combination of analytical and numerical techniques may be employed for the optimization of strongly perturbed soliton interactions. A comparison with the available experimental data will be also discussed.

YEW, Alice C (Ohio State University, USA)

Multiple pulses in dispersive quadratic media

Many models studied in modern optics take the form of two or more Schrödinger equations coupled together in a nonlinear fashion. Of special interest are solitary-wave solutions for which all of the components are localised in time (pulses in optical fibres) or in the space directions transverse to propagation (beams in waveguides). This talk is mainly concerned with a system describing second-harmonic generation and parametric wave interaction in dispersive quadratic media. In particular, the generation of multipulse solutions is demonstrated using methods from homoclinic bifurcation theory, and the stability properties of these multiple pulses are clarified analytically.

ZHARNITSKY, Vadim (Brown University, USA)

Stable pulse propagation in dispersion managed systems

We apply hamiltonian averaging to a system of ODEs obtained earlier by variational approach from the equation for electromagnetic pulse propagation in an optical waveguide. The minima and maxima of the averaged Hamiltonian correspond to the stable pulses. This is joint work with S Turitsyn, A Aceves, and C K R T Jones.

GOBBERT, Matthias K (University of Maryland, Baltimore County, USA)

A homogenization technique for a kinetic model for chemical vapor deposition

Chemical vapor deposition is used in the manufacturing of semiconductor chips to deposit thin layers of solid material on the surface of the wafer. The layer material is obtained from gaseous chemicals via surface reactions. Current numerical models all make the assumption of relatively high pressure regimes in order to use continuum equations. This assumption fails eventually as the integration of chip elements continues to increase. At the very low pressures in use, the mean free path of reacting gas particles in chemical vapor deposition is large compared to the typical dimension of the chip components. Thus, the flow must be described by a kinetic model. In this work, the velocities of the incoming particles are assumed to be a Maxwellian distribution on the reacting surface. Based on this ansatz, a homogenization technique yields an equivalent model that is more suitable for numerical simulations. This is a joint work with Christian Ringhofer.

JÜNGEL, Ansgar (Fachbereich Mathematik, Technische Universität Berlin, Germany)

Mixed finite-element discretizations of fluid dynamical models for semiconductors

The mixed exponential fitting finite element method is used for the discretization of quasi-hydrodynamic equations for semiconductors. The main idea of the discretization is to write the continuous problem in a drift-diffusion form and to employ local Slotboom variables. Two modern models for the simulation of semiconductor devices are presented: the isentropic drift-diffusion equations and the energy-transport equations. The first model is used to simulate 2D bipolar diodes and junction transistors. Ballistic diodes in 1D incorporating non-parabolic band structures are simulated by the second model.

KING, John R (University of Nottingham, UK)

Mathematical modelling of diffusion in compound semiconductors

Dopant diffusion in compound semiconductors is widely believed to be governed by highly nonlinear substitutional-interstitial mechanisms. Joint work with MG Meere involving the modelling of such processes will be outlined. Both asymptotic and numerical solutions of the models will be presented; in many cases the asymptotic approaches lead to novel (moving boundary problem) reformulations.

LEVERMORE, C David (University of Arizona, USA)

The zero dispersion limit of the NLS/mKdV hierarchy for the Nonselfadjoint Zakharov-Shabat operator

A numerical and theoretical study is presented of the zero dispersion limit for the focusing Zakharov-Shabat hierarchy, which includes NLS and mKdV flows. We establish the zero dispersion limit of all the nontrivial conserved densities for all of the odd flows in the hierarchy when the initial data is real-valued and reflectionless. In particular, this includes the mKdV flow, but not the NLS flow. The method is based on Lax-Levermore KdV strategy, but here it is carried out in the context of a nonselfadjoint spectral problem. The zero dispersion dynamics of the mKdV and that of the KdV become identical.

MUSCATO, Orazio (Dipartimento di Matematica, Catania, Italy)

Check of the consistency of carrier transport models in semiconductor devices with the Onsager reciprocity principle

The increasing miniaturization of modern electronic devices requires an accurate modeling of the energy transport in semiconductors, in order to avoid destructive phenomena in the device. Since a direct numerical integration of the full Boltzmann Transport Equation requires a heavy computational cost, simpler models have been exploited such as the Energy Transport Model, Hydrodynamic Model, Extended Hydrodynamic Model. In this paper we check the consistency of these models with the Onsager Reciprocity Principle, which is one of the fundamental principles of Linear Irreversible Thermodynamic. Monte Carlo simulations in the homogeneous and inhomogeneous cases are shown. This is a joint work with A M Anile.

ROMANO, Vittorio (Politecnico di Bari, sede di Taranto, Italy)

Hyperbolic hydrodynamical model for charge transport in semiconductors

The problem of the closure of the moment equations for the semiconductor Boltzmann equation is studied in the framework of the Kane dispersion relation. By using the maximum entropy ansatz for the distribution function of the charge carriers, one obtains, in the limit of small anisotropy, explicit constitutive relations for the stress tensor and the flux of energy flux tensor. Explicit expressions are also obtained for the moments of the collision term by taking into account electron scatterings with acoustic phonons, non-polar optical phonons and impurities. The closure relations are compared with those arising from Monte Carlo extraction of the transport coefficients and numerical results for ballistic diode are presented.

GRIGORIAN, Samvel S (Institute of Mechanics, Moscow Lomonosov State University, Russia)

On the predictive possibilities of mathematical models for determination of large-scale meteoroids nature

All the main mechanical and physical phenomena appearing in the course of big celestial body invasion in a planetary atmosphere are analysed and estimated quantitatively and corresponding mathematical models are constructed in the presentation. Numerical calculations based on these models demonstrate the predictive possibilities of such modelling.

KOROBENIKOV, Victor P (Institute for Computer Aided Design, Russian Academy of Sciences)

Simulation of celestial body desruption in the earth's atmosphere

The disruption of celestial body such as meteoroids, cometary fragments and asteroids is investigated by mathematical methods. The velocity of the body and its ablation during the first stage of the flight in an atmosphere are determined on the basis of the solution of the system of equations of the physical theory of meteors. The gas dynamic forces and radiation act on the body. The main results of the paper is related to the creation of stress-strain and phase transition models and simulation of the celestial body fracture and breaking up during its flight in an atmosphere. It was found that method of solution of thermoelastic equations (with prescribed boundary and initial conditions for a spherical body) by means of spherical functions series is appropriate for multi-variant calculations. A numerical algorithm was worked out and calculations were made. The practical convergence of the expansions were studied. An approximate analytical solution was obtained for the case of cylindrical body entering. The results are compared with those obtained numerically by finite element method. The phase transition of porous celestial body material under action of radiation is also studied by using of an energy equation and the mathematical catastrophe theory methods. The developed methods were applied to simulate the flight and disruption of icy bodies (fragments of comet heads), stone and metallic meteorites.

STULOV, Vladimir P (Institute of Mechanics, Moscow Lomonosov State University, Russia)

Deep impact: Mathematically modelling

A modern theory of meteor body motion in the atmosphere is described. Research of entry trajectories has shown that at large value of mass loss parameter, there are the rates when thermochemical destruction of the body proceeds faster than its deceleration. It results in that the body can undergo to full evaporation and continue motion as a jet of a mixture of vapor with ambient gas. Due to a large aerodynamic load at motion in the atmosphere, the meteoric body is subjected to mechanical destruction. Mathematical modelling based on the physical models of such destruction is developed. A series of analytical solutions allowing to present trajectories of debris clouds and some other properties of their motion in a simple kind, is submitted.

ALTENBACH, Holm (Martin-Luther-Universität Halle-Wittenberg, Halle, Germany)

On different approaches to the determination of the transverse shear stiffness in the plate theory

The classical Kirchhoff plate theory does not include constitutive equations for the transverse forces-transverse shear strains interactions. For thick, laminated and sandwich plates these equations have a significant influence on the correct estimation of the deflections or stress resultants and due to this fact we need refined theories. The quality of such theories depends on the correct determination of the stiffnesses. Many theories result in identical stiffnesses for bending, tension/compression, in-plane shear and torsion. In this contribution will be compared different proposals for the transverses shear stiffnesses.

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GOLDENVEIZER, Alexei L (Institute for Problems in Mechanics, Russian Academy of Sciences, Russia)

Approaches for refining 2D shell theories

Schemes for approximate construction of static shell theories are discussed. The methods utilised involve singular perturbation techniques for partial differential equations (The Prandtl scheme). It is established that the total stress-strain state of a shell may be decomposed into two parts, corresponding to propagating and exponentially decaying states. This motivates separation of the shell analysis into internal and edge calculations. The internal calculation employs Kirchhoff-Love theory, whilst the edge calculation requires solving the plane and anti-plane problems of elasticity in the vicinity of the edge. The scheme presented is a generalisation of both the Kirchhoff-Love and the Reissner-Timoshenko theories.

GREGORY, R Douglas (Dept. of Mathematics, University of Manchester, UK)

A thick hollow sphere compressed by equal and opposite concentrated loads; An asymptotic solution

An elastic *hollow* sphere with mid-surface radius R and thickness $2h$ is subjected to two equal and opposite concentrated loads acting at the ends of a diameter. The full three-dimensional solution to this problem consists of (i) a narrow Saint Venant component extending a distance of order $O(h)$ from each load point, (ii) a wider 'edge bending' component extending a distance of order $O(\sqrt{Rh})$, and (iii) a 'membrane' component which permeates the whole sphere. We determine the two outer components of the solution by a rigorously valid method which does not depend on Saint Venant's principle. We find an explicit two-term asymptotic approximation to this outer solution and make numerical comparisons between this refined theory, thin shell theory, and the Reissner-Wan theory.

HORGAN, Cornelius O (University of Virginia, USA)

Anisotropy induced singularities in linear elasticity

It has been known for some time that certain curvilinear anisotropies can give rise to stress singularities. An early example is due to E Reissner (J. Math. Mech. 7, 1958, 121-140) in the context of bending of orthotropic shells. Here we consider some linear elasticity problems where radial anisotropies lead to stress singularities which are absent in the corresponding isotropic problems. The problem of pressurized hollow cylinders and spheres is considered as well as problems for rotating disks. The anisotropies of concern here arise in the processing of fiber composites and in the casting of metals.

KAPLUNOV, Julius D (Institute for Problems in Mechanics, Russian Academy of Sciences, Russia)

Edge and interfacial vibrations of shells and plates

Vibration modes, localized near the edge of a shell (a plate), are studied. It is shown that the eigen spectrum of a shell of arbitrary shape consists of two subspectrums related to propagation of extensional and flexural Rayleigh-type waves. For a cylindrical shell there also exists the third subspectrum corresponding to super-low-frequency semi-membrane vibrations. The effect of shell geometry and boundary conditions, including their small imaginary parts caused by radiation to infinity, is investigated. The results obtained are extended to the case of the interface of a longitudinally non-homogeneous shell (a plate). Vibrations concerned with propagation of Stonely-type extensional and flexural waves are analyzed. This is a joint work with M V Wilde, Saratov State University, Russia.

KIENZLER, Reinhold (University of Bremen, Department of Production Engineering, Germany)

On consistent higher-order plate and shell theories

Plate and shell theories attempt to describe the three-dimensional state of deformation and stress in terms of the deformed and undeformed configurations of the middle surface. In this sense, plate and shell theories are inherently approximative. In the paper, all kinematic quantities are expanded in power series with respect to the thickness coordinate, while the dynamic quantities are replaced by weighted (thickness) averages. In turn, all field equations and boundary conditions are approximated uniformly. As results, a consistent, linear fourth-order plate and a second-order shell theory will be presented and compared to well-established classical theories.

KNOWLES, James K (California Institute of Technology, USA)

Shock-induced phase changes in solids

Experiments involving high-velocity impact on metallic or ceramic specimens are of interest in several fields, especially in geophysics, where such experiments are used to study high-pressure behavior of earth materials. Impacts generated in these experiments sometimes induce phase changes. This talk describes the application to impact-induced phase transitions of recently-developed continuum mechanical models of the macroscopic behavior of phase-changing solids. The role of transition kinetics in determining the material response is explored, and the task of inferring such kinetics from experimental results is briefly discussed.

KOSSOVICH, Leonid Yu (Saratov State University, Russia)

Flexural transient waves in shells of revolution: An asymptotic approach

The purpose of this paper is to present transverse asymptotic approximations for transient waves in thin walled shells of revolution initiated by edge bending shock loading. Equations for these approximations are derived by the method of asymptotic integration of 3D dynamic equations. Methods of solving the boundary value problems for the component considered are constructed with the help of Laplace transform, saddle point method and other ones. Methods obtained describe solutions for all values of time and show tending to static ones at increasing of time. This is a joint work with Ya A Parfenova.

LE, Khanh Chau (Lehrstuhl fuer Allgemeine Mechanik, Ruhr-Universitaet Bochum, Germany)

High-frequency vibrations of shells and rods: Variational-asymptotic approach

Two- (one-) dimensional equations are derived for high-frequency vibrations of linear elastic shells and rods. The derivation is based on the variational asymptotic analysis of the three-dimensional action functional. This guarantees the exactness of the derived equations for the classical and thickness branches of vibrations in the long-wave range. A best short-wave extrapolation is chosen so as to reach the qualitative agreement with the three-dimensional theory in the short wave range. A generalization to linear piezoelectric shells and rods is proposed. As an illustration dispersion curves, frequency spectra and edge modes are analyzed for circular plates, cylindrical shells and rods of the circular cross section. Comparisons are made with the similar results of the three-dimensional theory.

MARKENSCOFF, Xanthippi (University of California, San Diego, USA)

The mechanics of thin ligaments

In narrow regions of materials, such as between holes and free boundaries, or between inclusions, which we call thin ligaments, the stress amplifies singularly as the ligament thickness vanishes. The question that arises is how the stress relates asymptotically to the ligament thickness as it becomes vanishingly small. For many classical fibers in shear, etc. due to mathematical difficulties of the asymptotics of nonuniformly convergent series, it was not possible to obtain the limiting behavior of the stress and the question has remained open until recently. Actually this is a case where the numerical procedure also breaks down for very thin ligaments, because the number of terms required to be kept in the series for convergence exceeds the capacity of the computers. Singular asymptotics of series were developed and the limiting behavior of the stress as a function of ligament thickness was obtained. Comparisons with numerical evaluation are presented. The relation of the full field solution to the beam theory approximation of the thin ligaments is also discussed. Several examples of practical importance exhibiting stress amplification in thin ligaments under various loadings, including tension, pressure, body forces and thermal loadings are presented. Beam theory is used to determine the stress amplification in the thin ligaments in a strip containing an eccentric large hole. It is found that the stresses are inordinately larger than in the centrally placed hole due to higher bending moments transmitted through the ligaments.

ROGERSON, Graham A (Department of Computer and Mathematical Sciences, University of Salford, UK)

Some dynamic properities of idealised pre-stressed elastic plates

The dispersion realtion associated with small amplitude waves propagating in an idealised (inextensible and incompressible) elastic plate is derived in respect of the most general appropriate strain energy function for propagation along a non-principal diection. High and low wave number approximations, giving phase speed as a function of pre-stress, wave number and harmonic number, are derived and compared with numerical solutions. Conditions for both the existence of surface waves and loss of infinitesimal stability are also derived.

SIMMONDS, James G (Univ. of Virginia, Charlottesville, USA)

Computing exact, elastodynamic linear three-dimensional solutions for plates from classical two-dimensional solutions

Given a three-dimensional formulation for an initial/boundary value problem for a platelike domain in three-dimensional elasticity, it is shown how, starting from a solution of the classical (Kirchhoff) theory of plates, one may construct an exact, time-dependent solution of a "neighboring" three-dimensional problem. A novel feature of the analysis is that the problem reduces to solving an integral equation (the consistency condition) which arises in turn from solving a hyperbolic wave equation in which the role of the "time" variable is played by the thickness coordinate while the actual time enters only as a parameter.

SPENCER, Anthony J M (University of Nottingham, UK)

Exact solutions for inhomogeneous thick elastic plates

A large class of exact solutions is derived for stretching and bending of thick elastic plates which are inhomogeneous in the through-thickness direction. Essentially, any solution of the classical two-dimensional thin plate equations generates an exact three-dimensional elasticity solution for an inhomogeneous thick plate. Laminated plates are included as a special case.

STEIGMANN, D (University of California, Berkeley, USA)

On the relationship between the Cosserat and Kirchhoff-Love theories of elastic shells

We clarify the relationship of the Kirchhoff-Love theory of elastic shells to the more general Cosserat theory of deformable surfaces with a single director. The latter has as its kinematical basis two vector fields defined on the surface, one that defines the particle position, and the other, the director, that is intended to account for finite-thickness effects. Specifically, we obtain the Kirchhoff-Love theory by imposing constraints on the director field and deriving the general forms of the associated response functions through a careful application of the rigorous Lagrange multiplier rule. Although this rule is standard, the constraints considered are of an unusual type and the development thus includes more detail than one usually finds in the literature on constrained elasticity. In Naghdi's treatment of the subject the Kirchhoff-Love theory is not derived from the Cosserat theory but instead is considered separately on the basis of distinct balance and invariance postulates. This contrasts with our view that the Cosserat theory should reduce to the Kirchhoff-Love theory upon the introduction of appropriate constraints. There are additional differences between Naghdi's treatment and ours. For example, his relies on the moment-of-momentum equation to determine the skew part of a tensor whose symmetric part alone is deemed to be constitutively determinate. However, in conventional finite elasticity theory the moment-of-momentum equation is identically satisfied if the strain energy is invariant under superposed rigid motions. In the present work the response function in question is shown to be fully determinate and the moment-of-momentum equation reduces to an identity for invariant strain energies. Further, in Naghdi's treatment the constitutively indeterminate skew part of another tensor that furnishes the moments transmitted across material curves is arbitrarily set to zero to obtain a determinate system of equations. We show this to be unnecessary. Nevertheless the resulting model is substantially equivalent to Naghdi's, and thus the differences between the two approaches are primarily conceptual, the main distinction being that the logical framework of the present development conforms to that of finite elasticity theory.

WAN, Frederic Y M (University of California at Irvine, USA)

The outer asymptotic expansion solution without matching

For many singular perturbation boundary value problems in partial differential equations, the method of matched asymptotic expansions is applicable in principle but not feasible in practice. The difficulty often lies in that the inner (asymptotic) solution needed to fit the boundary data is difficult to obtain in terms of known functions. The present paper describes a method for finding the correct outer (asymptotic) solution of linear boundary value problems without any reference to the inner solution. The method is based on the requirement that the difference between the exact and outer solution of the problem (called the residual state) must be rapidly decaying. New results will be presented to address the relevant uniqueness issue for this method of decaying residual state (DRS). For applications to solid mechanics, the classical Saint Venant's principle in linear elasticity theory will be deduced as a special consequence of the general method of DRS and results for boundary value problems in elastostatics for which Saint Venant's principle does not apply will also be reported.

ZAKHAROV, Dmitrii (Institute for Problems in Mechanics, Moscow, Russia)

Boundary value problems for composite laminates under bending-extension coupling

On the basis of 2D asymptotically accurate model of thin composite laminate with arbitrary anisotropy and layup, the boundary value problem (BVP) for the internal stress-strain state is studied. The peculiarity of the problem consists in the coupling of bending and stretching processes, where classical plate problems of bending and of in-plane stress state are particular cases. For the analytical solution to the coupled BVP four generalized potentials are introduced. Their properties are similar to those of the familiar Kolosov-Muskhelishvili-Lekhnitskii potentials, and to the Stroh formalism. Thus, the first and second BVP are reduced to the problem of complex analysis: to find out a set of functions inside the region by known values of some expressions with these functions on the boundary. The conditions of single values for the physically meaningful functions are deduced, as well as the conditions of total integral equilibrium. For the not self-equilibrated loads (or for the fundamental solutions) the corresponding logarithmic potentials are found out. It is shown, that in our case the set of analytical solutions embraces all the cases of the plate regions, where the solution of separate bending or stretching problems are known. Some examples for the canonical regions (semi-plane, strip, wedge, internal or external ellipse, crack or rigid inclusion in a plane, etc.) are presented. For the more complicated shape of plate region the system of boundary integral equations is deduced and analysed. This work was partially supported by DFG (German Research Foundation), project BE 1090/5-1, which is gratefully acknowledged. This is joint work with Dmitrii D Zakharov and Wilfried Becker.

BÉNARD, Marc (Université de Strasbourg, France)

Algorithmic and numerical challenges in today's computational quantum chemistry

New algorithms have been recently designed for the calculation of the Coulomb and exchange parts of the electron repulsion matrix which lead to a linear scaling for the calculation of the Fock matrix. Applying those methods to large systems shows that diagonalization, even using Lanczos-type algorithms, soon becomes the most time-consuming step. A diagonalization-free quantum chemistry is therefore being developed which allows for complete linear scaling and parallelization of ab initio and DFT SCF iterations. Examples of calculations will be presented to illustrate the possibilities of those algorithms and the perspectives of ab initio quantum chemistry in the near future.

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BLANC, Xavier (Ecole Nationale des Ponts et Chaussées, France)

On the algorithms in use in the simulation of the solid phase

We will present a broad overview of the numerical algorithms used for the simulation of the crystalline phase. Questions of convergence will be carefully examined. We will also lay some emphasis on open problems.

BOKANOWSKI, Olivier (Université Paris 7 and Paris 6, France)

High density limits to the Thomas-Fermi-von Weizsäcker-Dirac model via deformations of plane waves

We deal with local density approximations for the kinetic and exchange energy terms of an Hartree-Fock type model of an N -electron system. Our method is based on "deformations" of plane waves (in a cubic box with periodic boundary conditions) and the "high density" limit of infinite number of particles. For the first order approximation of the kinetic energy, we give a derivation of the usual combination of the von-Weizsäcker term and the Thomas-Fermi term. We also show how to obtain the Slater-approximation where the exchange term is replaced by the third root of the local density.

CAFFAREL, Michel (CNRS, Université Paris VI, France)

Solving the Schrödinger equation with probabilistic methods: Quantum Monte Carlo and quantum chemistry

In recent years probabilistic methods for solving the Schrödinger equation (also referred to as Quantum Monte Carlo methods) have become a subject of increased interest in quantum Chemistry. In this presentation I will briefly review the main formulations of QMC and present the basic mathematical aspects common to all approaches. A number of selected applications will be presented to exemplify the basic ideas and to illustrate how successful quantum Monte Carlo can be for certain systems. Finally, I will discuss the limitations of these methods and present some open mathematical problems.

CANCES, Eric (CERMICS, Ecole des Ponts, France)

On the convergence of SCF algorithms for the Hartree-Fock equations

The present work is a mathematical analysis of two algorithms, namely the Roothaan and the level-shifting algorithms, commonly used in practice to solve the Hartree-Fock equations. The level-shifting algorithm is proved to be well-posed and to converge provided the shift parameter is large enough. On the contrary, cases when the Roothaan algorithm is not well defined or fails in converging are exhibited. These mathematical results are confronted to numerical experiments performed by Chemists.

CATTO, Isabelle (CNRS & CEREMADE, Université Paris-Dauphine, France)

Hartree-Fock type models for crystals

In this talk, we shall present mathematical results recently obtained on Hartree and Hartree-Fock type models for crystals. By the way, we shall also explain how we have derived (or guessed) these models from well-known models for molecules in Quantum Chemistry, by using the so-called thermodynamic limit.

This is a joint work with C Le Bris and P-L Lions.

COULAUD, Olivier (Inria-Lorraine & Iecn)

Numerical simulation in biological molecular systems

Numerical simulation in biological molecular systems requires to take into account solvent to modelize the environment surrounding the protein. A classical modelization is to consider explicitly the solvent (for molecule of water we have three atoms) and then, this leads to a simulation with a large number of atoms (greater than 100 000). The evaluation of the electrical potential is the bottle-neck in such simulation. An other modelization, is to consider explicitly only a small number of solvent molecules near the protein and the electrical behaviour of the solvent on the protein is modeled by an electrical continuum. For this method, we will present an efficient method based on an integral formulation on the molecular surface for solving the potential and the electrical field. After that, we will give an algorithm to couple the continuum approach with the molecular dynamic, finally results on Origin2000 will be given.

DEFRANCESCHI, Mireille (Commissariat à l'Energie Atomique, France)

Examples of quantum mechanical calculations of condensed phase

This contribution highlights that chemistry is a macroscopic science but its foundation rests in the atomic scale, in the interplay between the motions of the nuclei and the distribution of the electrons. For long, the solution of the fundamental equation of quantum mechanics, namely Schrödinger's equation, seemed far too complicated for even simple systems. The recent improvements of both theory and computation capabilities have made possible to solve the equation for materials. A survey of various methods will be given. The discussion of specific computational methods such as all-electron localized basis approaches, pseudopotential plane methods constitute the central part of the presentation. Practical examples on real materials will be included.

ESTEBAN, Maria J (CEREMADE, CNRS and Université Paris IX-Dauphine, France)

Min-max characterization of energy levels in relativistic atoms

In this talk we give two different variational characterizations for the eigenvalues of $H + V$ where H denotes the free Dirac operator and V is a scalar potential. The first one is a min-max involving a Rayleigh quotient. The second one consists in minimizing an appropriate nonlinear functional. Both methods can be applied to potentials which have singularities as strong as the Coulomb potential.

KRESSE, Georg (Institut für Materialphysik, Universität Wien, Austria)

VASP: An efficient and versatile plane wave pseudopotential program

First principle calculations based on the Kohn-Sham density functional theory are used by an ever increasing number of scientists to predict chemical and physical properties of materials. Although many elaborated packages exist to predict the behavior of small molecules, programs that are capable of treating extended systems like metal surfaces or zeolites - materials which are important for industrial catalysis - are still rare. To meet this demand, a powerful package called VASP (Vienna ab initio program) was developed over the last few years (see G Kresse and J Furthmüller, Phys. Rev. B **54**, 11169 (1996) and <http://tph.tuwien.ac.at/vasp/>). It utilises plane waves and periodic boundary conditions and allows model systems containing around 100 atoms to be studied on workstations. The interactions between ions and electrons are described by the projector augmented wave method (see P E Blöchl, Phys. Rev. B **50**, 17953 (1994)) or pseudo potentials. In the lecture a brief description of the essential ideas underlying the pseudo potential approximation and plane wave basis set are given. Then the algorithms implemented in VASP are discussed in more detail and compared to other existing methods. It is shown that our present algorithms are very stable for a wide class of materials, scale extremely well with system size and can be parallelized efficiently even on small clusters of personal computers.

LE BRIS, Claude (Ecole Nationale des Ponts et Chaussées, France)

On the TDHF equations

With a view to attacking problems of control theory in Quantum Chemistry, we present the rigorous mathematical foundations of the time dependent Hartree-Fock equations, and some related equations. We also present a broad overview of the models in use for the simulation of time-dependent phenomena.

LE TALLEC, Patrick (Université Paris Dauphine, France)

Mesoscopic modelling of polymers

The purpose of the talk is to describe the difficulties encountered in the mathematical simulation of polymers at a mesoscopic scale. A first problem is to derive the macroscopic material properties of a polymer from a statistical knowledge of the elementary chains of which it is made. Because of the numerous geometrical constraints and of the time scales involved, computing these statistical data by direct simulation seems out of reach. The next problem is to build and integrate an adequate kinetic model to compute the resulting equilibrium configurations, taking into account both elastic and plastic effects.

MADAY, Yvon (Laboratoire ASCI-CNRS, Orsay, France)

Error estimators for the approximation of the solution of Schrodinger's type equations

The numerical simulation of the equations derived from the Schrodinger equations for problems of interests in quantum chemistry most often leads to the resolution of discrete equations with very large size. Even though "computational chemists" know the good basis that have to be used in order to minimize at most the computational cost, there is a need of theoretical tools that can provide some reliability for the conclusion of the computations. With Gabriel Turinici, we have developed some tools that enter in the category of *error estimators* that allow for giving some precise and reliable information on a certain number of calculations. In this talk we shall present these tools so as numerical simulations that illustrate their efficiency.

MENNUCCI, Benedetta (Università di Pisa, Italy)

Quantum mechanical models for systems in solution

In the last few decades the main efforts in the chemical research have been addressed to the study of condensed phases, generally liquid solutions. That has led to the formulation of various theoretical models of very different nature. With the present contribution we shall try to give a necessarily limited view of the state of art in this research field, including the main challenges for the future. In particular, the attention will be focussed on one of the possible strategies, namely the continuum approximation. In this scheme only a limited portion of the whole system, the solute, is described quantum-mechanically while the main part, the solvent, is treated as a continuum distribution, without microscopical nature, but acting as an additional perturbation to be introduced in the Hamiltonian of the solute in vacuo.

RAYBAUD, Pascal (Institut Français du Pétrole (IFP), France)

Ab-initio calculations applied to heterogeneous hydrodesulfurization catalysis

Heterogeneous hydrodesulfurization catalysts are used in industrial processes to remove sulfur or other heteroatoms from petroleum cuts. Under working conditions the active phase of these catalysts are mixed - Transition Metal Sulfides (TMS). The precise understanding of the TMS reactivity is still an open question. Calculations within the DFT-GGA formalism as implemented in the "Vienna Ab-initio Simulation Package" (see G. Kresse's MSP) provide a powerful way of investigation. The structural, electronic and energetic fundamental properties of TMS realistic models are determined in order to point out relevant parameters that may correlate with the TMS experimental catalytic activity.

This is a joint work with H Toulhoat, Institut Français du Pétrole (IFP), J Hafner and G Kresse, Technische Universität Wien (TUW).

SAUE, Trond (IRSAMC, France)

Quaternion symmetry in relativistic molecular calculations

A quaternion formulation of the time reversal symmetric one-electron Dirac equation and many-electron Dirac-Fock equation is presented. This formulation provides automatically maximum point group and time reversal symmetry reduction of the computational effort, also when the Fock matrix is constructed in the scalar basis, that is, from the same type of electron repulsion integrals over scalar basis functions as in non-relativistic theory. An illustrative numerical example is given showing symmetry reductions comparable to the non-relativistic case.

SERE, Eric (CEREMADE, Université Paris IX-Dauphine, France)

Solutions of the Dirac-Fock equations

The Dirac-Fock equations are the relativistic analogue of the well-known Hartree-Fock equations. They are used in computational chemistry, and yield results on the inner-shell electrons of heavy atoms that are in very good agreement with experimental data. By a variational method, we prove the existence of infinitely many solutions of the Dirac-Fock equations "without projector", for Coulomb systems of electrons in atoms, ions or molecules, with $Z \leq 124$, $N \leq 41$, $N \leq Z$. Here, Z is the sum of the nuclear charges in the molecule, N is the number of electrons.

SUTCLIFFE, Brian T (Lab. de Chimie Phys. Moléculaire, ULB, Bruxelles, Belgium)

Is a molecule in chemistry explicable as a broken symmetry in quantum mechanics?

The Schrödinger equation for a collection of nuclei and electrons that a chemist might regard as constituting a molecule does not actually define a unique chemical object. To realise the required solutions for the desired molecule seem to require the imposition of certain mathematical constraints on the equations. These constraints will be discussed with particular attention paid to a constraint that breaks the symmetry of the problem. A discussion will be opened on whether such constraints might be avoided.

TURINICI, Gabriel M (Laboratoire ASCI-CNRS, Orsay, France)

Quantum control of chemical reactions

Controlling chemical reactions at the quantum level was a long-lasting goal for the chemists from the very beginning of the laser technology. Experience showed that designing the laser pulse able to steer the system to the desired target state is a rather difficult task that physical intuition alone cannot accomplish. It is only recently that tools coming from control theory began to give satisfactory results in some particular cases; finding the optimal electric field is now treated by numerical methods and new models are sought after that be also reliable and cheap from a computational point of view. The purpose of our talk is to give an insight into this emerging field through a presentation that include both an outline of those topics and also some of our joint work with Professor Yvon Maday.

GREENBAUM, Anne (University of Washington, USA)
Comparison of QMR-Type Methods with GMRES

Several iterative methods for solving linear systems construct basis vectors for a sequence of Krylov subspaces and then choose approximate solutions from among these basis vectors by minimizing the residual norm in a reduced least squares problem. We refer to methods that solve the reduced least squares problem as QMR-type methods, regardless of the recurrence used to construct the basis vectors. It is known that if the basis vectors are well-conditioned then the approximate solution obtained in this way is reasonably close to the optimal approximation from the Krylov subspace. We extend this result to show that if some subset of the basis vectors are well-conditioned, and if the GMRES residual from some earlier step can be well-approximated in the space spanned by this subset of vectors, then the residual norm for the QMR-type method is closely related to the GMRES residual norm at this earlier step.

HANKE, Martin (Fachbereich 17 Mathematik, Johannes-Gutenberg-Universität Mainz, Germany)
Semiiterative regularization methods for ill-posed indefinite problems

We consider linear equations with a selfadjoint and indefinite linear operator. Such equations are called ill-posed if the spectrum of the linear operator clusters in the origin, and therefore, the solutions do not depend continuously on the given right-hand sides. Assuming that the spectrum of the linear operator is contained in the interval $[a, 1]$ where a is some given negative real number we construct semiiterative methods for the efficient numerical solution of the linear system based on short recurrences. The main tool are kernel polynomials corresponding to a generalized Jacobi weight over the interval $[a, 1]$. This is joint work with Harald Frankenger, Universität Kaiserslautern.

HUHTANEN, Marko T (Helsinki University of Technology, Finland)
 $[A, A^*]$ and inversion of the sum operation in $A = \text{normal} + \text{small rank}$

Suppose a given $A \in \mathbb{C}^{n \times n}$ is known to be a sum $A = N + F$ of an *unknown* normal matrix N and an *unknown* rank- k matrix F with $k \ll n$ and the task is to find F . This type of "inverse problem" is related to an analysis of the behaviour of iterative methods for A . In this talk we show that if $\text{rank}(F) \leq \lfloor \frac{\text{deg}(N)}{4} \rfloor$, then, generically, the resulting sum $A = N + F$ yields a *minimal decomposition* of A . Furthermore, we show that, generically, F can be found by using the self-commutator $[A, A^*]$ of A . More precisely, the problem of finding F is related to construction the solution set of $[Z, Z^*] + [A_W^*, Z] + [Z^*, A_W] = -W^*[A, A^*]W$ for Z with matrices of size at most $4k$ and W has at most $4k$ orthonormal columns that span the range of $[A, A^*]$.

KELLEY, Carl T (North Carolina State University, USA)
Convergence behavior for Krylov space linear solvers: Examples and applications

Krylov methods are often applied in situations where only the matrix-vector product can be approximated (ie a full matrix is not available). Typically the matrix-vector product function has errors. Examples are truncation error when discretizations of infinite dimensional problems are being solved, differencing error when Jacobian-vector products are approximated by differences, and internal errors that arise when routines used inside the matrix-vector product have errors, perhaps under user control, that propagate into the matrix vector product. In this talk we will discuss both theoretical and practical aspects of managing the iteration in the presence of these errors. Examples will be taken from nonlinear equations, numerical bifurcation, and optimization.

NEVANLINNA, Olavi (Helsinki University of Technology, Finland)
Resolvent as a meromorphic function

We show in this talk how viewing the resolvent of a matrix as a meromorphic function can be used to explain convergence phenomena of Krylov methods. In the "usual" analysis one treats the resolvent as an analytic function outside the spectrum, and hence such an analysis is always sensitive to, say, low rank perturbations. In contrast, if the resolvent is measured as a meromorphic function, then the "size" or "growth" of the resolvent is insensitive in low rank perturbations. With this approach we can give upper bounds for the error of GMRES which are robust in low rank perturbations.

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FASANO, Antonio (Dept.Math. "Ulisse Dini", University of Florence, Italy)

Fuels with peculiar rheological properties

Some fuels exhibit a highly nonlinear behaviour, characterized in most cases by a dependence of some or all the rheological parameters on the history of the flow. A typical case is the one of coal-water slurries (CWS), i.e. highly concentrated mixtures (up to 70% by volume) of finely ground coal with water, with the addition of a small amount of a fluidizing agent. The dynamics of CWS has been the subject of an intense cooperation with Snamprogetti which lead to the interpretation of the so-called rheological degradation and to the formulation of a model describing the complex phenomenon of sedimentation of impurities. We have a completely different picture for diluted suspensions of coal in water, posing entirely different questions, like e.g. phase separation. Another remarkable example is the pipelining of waxy crude oils (oils with high content of paraffin), whose peculiar flow properties at low temperatures must be attributed to the crystallization of paraffin and the agglomeration of crystals. One more interesting problem is the flow of liquid-liquid dispersions. In addition to phase separation, here we have the interesting problem of the evolution of liquid-liquid dispersions under controlled shear rate, for which a new model is proposed, accounting for the existence of a top admissible size for the dispersed drops, depending on the strain rate.

ROSSO, Fabio (Dept.Math. "Ulisse Dini", University of Florence, Italy)

Dynamics of liquid-liquid dispersions

A liquid-liquid dispersion is a mechanical system formed by a population of droplets of variable size of a given component A finely distributed into another component B immiscible with A. The two phases can generally interact thermally and chemically, besides mechanically, but we will not consider this complication here. These systems are rather common in important industrial and environmental applications such as colloid chemistry, dense crude oil extraction and pipelining, photographic processes, meteorology. Rational design of dispersed phase reactors requires a knowledge of the evolution of the size distribution function, which is. We present a new model for the evolution equation in which we introduce some features in order to take into account an important experimentally observed fact: the reactor geometry and the shear rate imposed to the system through the impeller, determines the top size limit of the droplets. Unlike other models, which consider only coalescence and breakage interactions, we add a *volume scattering term* preserving the total number of droplets during interaction, and an *efficiency function* depending on both the total number of droplets and the total interfacial area and controlling the time rate of all kinds of interactions. The simultaneous action of the scattering term and of a cut-off imposed to the coalescence kernel prevent the appearance of "too large" droplets. Indeed coalescence gives rise to droplets that have a non-zero average life time and therefore has to be set to zero when coalescence would produce a too large droplet. On the other hand, volume scattering allows the formation of a *virtual* large droplet that does not survive and decays into a pair of droplets within the admissible volume range. We prove the physical consistency of the model and a global existence - uniqueness theorem for the evolution equation which governs the droplet size distribution function.

SONA, Giuliano (Dept.Math. "Ulisse Dini", University of Florence, Italy)

A mathematical model for gravity phase separation in liquid-liquid dispersions

In many oil industry is sometimes necessary to separate multiphase dispersions (oil-water-gas) generated during enhanced oil recovery in off-shore platforms. Indeed this water is generally salty, radioactive, or rich of ionized particles which, if the product is pipelined without any treatment, can cause severe problems like pipe wall corrosion, explosion and hazards. Under the action of gravity, a multiphase dispersion left at rest in a container will finally turn out to be fully separated in neatly distinct phases. We developed a mathematical model for gravity driven phase separation based on monitoring the evolution of the *hold-up* function (content by percentage) of the dispersed phase. The analysis leads to a system of first order PDEs which is proved to be strictly hyperbolic.

SPERANZA, Alessandro (Dept.Math. "Ulisse Dini", University of Florence, Italy)

Pipelining of diluted coal-water suspensions

Transport of mixtures of ground coal with water can be performed using two different technologies: concentrated suspensions (slurries, up to 70% by volume of coal content), diluted suspensions (coal concentration of the order of 50%). The physical properties of the two systems are basically different. A mathematical model for diluted suspensions pipelining is presented with phase separation. The fresh suspension introduced in the pipeline is subjected to partial segregation due to gravity. The dynamical model describes the evolution of three phases. The bulk of the suspension occupies the upper layer, the intermediate layer is a denser suspension, the bottom layer is a solid sediment. Mass transfer occurs according to a specific kinetics from upper to lower layers. The solid concentration and the thickness of the intermediate dispersion are fixed. There is also a transient stage in which the solid sediment (whose presence should be at least delayed) is absent. This picture is suggested on one side by the existing models of multiphase flows and on the other hand by the successful approach to the analysis of sedimentation in coal-water slurries, in which the presence of the intermediate moving layer is a key feature for a correct prediction of the dynamic behaviour of the plant.

TERENZI, Alessandro (Snamprogetti, BAPAC Dept., Italy)

Transient compressible flow at high mach numbers: A conservative method for pipeline flow

A computer code called Machnet has been developed to predict phenomena occurring during transient phases associated with gas pipeline flow at high Mach numbers. Vessels and pipelines rapid depressurizations are representative examples of this fluid mechanics condition. The code is based on a one-dimensional conservative approach derived from the Godunov scheme, with a first order explicit time integration. It includes a treatment of friction and heat exchange effects along with a description of valves and orifices installed in the pipes. Sections changes are analyzed also, and the boundaries are simulated considering their real shape within the numerical method used for the interior cells, without resort to characteristics. The adapted thermodynamic model refers to the perfect gas scheme with correction factors taking care of real behaviour. Comparisons are shown between Machnet simulations and analogous calculations from other programs, or with available experimental data also.

BENAMOU, Jean-David (INRIA-Rocquencourt, France)

Computation of generalized Monge-Kantorovich distances

The L^2 Monge-Kantorovich mass transfer problem is reset in a Fluid Mechanics framework. We now look for an "optimal" time dependent flow transporting the mass between prescribed initial and final mass densities. These new time dependent unknowns solve a convex minimization problem with linear constraints. They also provide a natural continuous time interpolant between initial and final mass densities. Numerical results will be presented. They are obtained using either an augmented Lagrangian technique for saddle point problems or, after a relaxation leading to an optimal control problem, a conjugate gradient algorithm.

This is joint work with Y Brenier.

BRENIER, Yann (IUF and University Paris 6, France)

Kantorovich distance and particle schemes

The Monge-Kantorovich (or Wasserstein) distance is a useful concept to understand apparently unrelated numerical schemes using particles. This includes a particle scheme introduced by G Russo for the heat equation, a scheme for a stiff version of the Vlasov-Poisson system (in the so-called quasi-neutral regime), recently introduced by Y Brenier, and some of the numerical schemes introduced by the UK meteorological office for semigeostrophic flows.

CULLEN, Michael J P (ECMWF, UK)

Applications of the Monge transport problem to meteorology and oceanography

It is shown how the 'semigeostrophic' equations are an appropriate approximation to the equations of motion of the atmosphere and ocean when rotation and stratification are strong. It is shown how these equations can be formulated as a coupled Monge transport and evolution problem, and under what conditions the Monge transport part can be solved. In the special case of constant rotation, the problem becomes a coupled Monge Ampere/transport problem. Solutions for this case are exhibited, including discontinuities which are a model of atmospheric fronts. Finally, applications of Monge transport theory to forecast verification are discussed.

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MSP-070

GANGBO, Wilfrid (Georgia Institute of Technology, USA)

Uniqueness of equilibrium configurations in solid crystals

Despite that $M \rightarrow h(\det M)$ is not coercive, we prove that the functional $E[\mathbf{u}] := \int_{\Omega} (h(\det D\mathbf{u}) - \mathbf{F} \cdot \mathbf{u}) dx$ admits a unique minimizer over the set \mathcal{U}_{Λ} of all orientation-preserving deformations $\mathbf{u} \in C^1(\Omega)^d$ that are homeomorphisms from $\bar{\Omega}$ onto $\bar{\Lambda}$ provided that $\det DF$ is positive, h is strictly convex of class $C^2(0, +\infty)$, satisfies suitable growth conditions at 0^+ and $+\infty$ and $\mathbf{F}(\Omega)$, Λ are convex. This is done by introducing a relaxation of $\inf_{\mathcal{U}_{\Lambda}} E$ and identifying a problem dual to the relaxed problem. Next, given $\mathbf{u}_o \in \mathcal{U}_{\Lambda}$ we study the pure displacement boundary value problem that consists in minimizing E over \mathcal{U}_o the set of maps $\mathbf{u} \in \mathcal{U}_{\Lambda}$ with prescribed boundary values \mathbf{u}_o . We show that the infimum of E over \mathcal{U}_{Λ} and \mathcal{U}_o coincide and conclude that in general the pure displacement boundary value problem does not admit a minimizer.

MCCANN, Robert J (University of Toronto, Canada)

Optimal transportation on manifolds with obstacles

With Mikhail Feldman (of Northwestern University), we consider optimal transportation of mass in a curved landscape around a convex obstacle. That is, given two distributions of mass, we construct an optimal map which rearranges one distribution into the other while minimizing the average distance shipped and avoiding the obstacle. Degeneracies associated with the convergence of geodesics on the obstacle boundary are resolved using a measure decomposition obtained explicitly.

BENAMOU, Jean-David (INRIA-Rocquencourt, France)

Direct computation of phase-space multivalued solutions of the Eikonal equation

Ray solutions of the Eikonal equations are classically computed using the bicharacteristics. The bicharacteristics actually span a Lagrangian submanifold in phase-space which, when folded, projects to a multi-valued solution onto configuration space. Our algorithm automatically computes this multi-valued solution without shooting the bicharacteristics. It uses finite-difference solutions of a coupled Eikonal/Transport system of equations. It also relies on the a priori knowledge about the generic structure of the folds in phase-space to unfold the Lagrangian submanifold into several single valued solutions of the Eikonal equation.

BRENIER, Yann (IUF and University Paris 6, France)

Moment methods for the Eikonal equation

The computation of multivalued solutions of the eikonal equation, on a finite difference grid in the physical space using CFD solvers, has been addressed by several authors in the recent years. In the present talk, we show that, provided an a priori bound is known for the number of branches N , the moment equations obtained from the corresponding Liouville equation set in the phase space can be closed at a finite order M and the resulting system of non-linear (degenerate) hyperbolic equations can be solved by classical CFD finite difference schemes in the physical space. This idea has been also used by B Engquist and O Runborg. If M is not chosen large enough, there is a discrepancy between the exact solution and the moment solution, that can be analyzed following the ideas of Y Brenier and L Corrias, published in Ann. IHP Analyse non-lineaire, 1998.

ENGQUIST, Bjorn (UCLA, USA and NADA KTH, Sweden)

Application of level set techniques in geometrical optics

The level set method has been used for a great number of problems involving propagating fronts. It has been particularly successful for problems where the physics dictate that meeting fronts should merge to create topology changes. We will show some new ways of using methods of level set type also in problems where meeting fronts should overlap, such as in geometrical optics. Applications include direct solution of the eikonal equation with multiple phases and ray tracing.

RUNBORG, Olof (NADA KTH, Sweden)


New results in multiphase geometrical optics

In order to be able to capture solutions containing multiple phases we formulate geometrical optics as a kinetic transport equation set in phase space. If the maximum number of phases is finite and known a priori we can recover the exact multiphase solution from an associated system of moment equations, closed by an assumption on the form of the density function related to the transport equation. We compare the analytical and numerical properties of the resulting equations for two different closure assumptions; when the density functions is a sum of delta functions and of Heaviside functions.

BOARDMAN, Allan D (University of Salford, UK)

Dynamics of non-Kerr solitons - A new approach

The dynamics of solitary waves in second-order nonlinear materials are discussed. An approach is developed with a view to setting up a line of approach that permits radiative effects to be modelled. The evolution of dynamical variables is developed. Applications of this novel approach are presented together with confirmation from numerical simulations. It is emphasised that the method is capable of extension to higher-order perturbations and into the solitary wave fusion region. The interpretation of quasi-phase-matching fluctuations, pair interactions in both loss-free and lossy/amplifying media are analysed.

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 MSP-073

FIRTH, William (University of Strathclyde, Glasgow, UK)

Stability, control and manipulation of nonlinear optical patterns

Many nonlinear optical systems can produce spontaneous output patterns. We present analytical and numerical techniques for the identification and generation of such patterns and their stability. These techniques lead to experimentally realisable (and realised) schemes for their control and stabilisation. By suitably filtered feedback we are able to dynamically select exact hexagonal, striped, square and unpatterned states in a minimally-invasive manner. We also discuss the existence, stability, and manipulation of localised pattern elements for applications in information processing. This work has been performed in collaboration with G.-L. Oppo, G.K. Harkness and others, and is supported by EPSRC grant GR-J 19727 and ESPRIT project 28235 - PIANOS.

FISHMAN, Louis (Naval Research Laboratory, USA)

Phase space and path integral methods in integrated optics

Wave propagation in inhomogeneous and nonuniform guiding structures is a central theme in integrated optics. For fixed-frequency formulations, the parabolic equation (PE) method (also known as the BPM in the optics literature) provides one-way approximations to elliptic models such as the Helmholtz equation. The application of phase space analysis, path integral techniques, and exact, well-posed, one-way reformulations based on Dirichlet-to-Neumann operators extends the traditional PE methods to the general, two-way problem. This results in phase space marching computational algorithms, the generalized Bremmer coupling series, and several natural approaches to corresponding inverse scattering formulations.

SHENG, Qin (University of Southwestern Louisiana, USA)

On a spline collocated difference method for the nonlinear Schrödinger equation

This talk is concerned with a second order finite difference method for solving the nonlinear Schrödinger equation. The numerical scheme is constructed through a collocation of the cubic spline approximation. Homogeneous Neumann boundary condition is employed in the discretized problem and second order forward/backward differences are considered for approximating the boundary values. The near conservation criterion is introduced to ensure the conservative property of the numerical scheme. We also discuss conservative and nearly conservative properties for several well known schemes in the literature. The stability of the numerical method developed is studied. Our investigation reveals an efficient and reliable way for computing the solitonian solution of the nonlinear Schrödinger equation. Numerical examples are given to further demonstrate our results.

STRUTHERS, Allan A (Michigan Technological University, USA)

Three wave interaction solitons in optical quadratic frequency conversion processes

Three Wave Interactions (TWI) are fundamental in laser science and technology: they generate different frequencies from readily accessible laser sources. More recently they have also been used to compress pulse and proposed as candidates for all-optical switching. An Inverse Scattering Theory (IST) for the TWI was developed in 1976. Until recently this IST had not been applied to describe and improve the numerous optical processes described by the TWI. This talk outlines the TWI scattering theory, describes analytical implications of the scattering theory for several common nonlinear frequency conversion techniques, and sketches some novel applications of TWI interactions suggested by the analysis.

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MSP-074

COCKBURN, Bernardo (School of Mathematics, University of Minnesota, USA)

Discontinuous Galerkin methods for convection-diffusion problems

We present the Local Discontinuous Galerkin (LDG) method for convection-diffusion problems. The main feature of this method is that it uses discontinuous approximate solutions. This allows a high parallelizability of the scheme and a great ease in performing 'hp' adaptation; it also allows the scheme to be stable for all values of the diffusion coefficients, even for diffusion coefficients equal to zero. We present the method, discuss its computational advantages, and discuss its accuracy. The LDG method was developed with Chi-Wang Shu of Brown University. This work was partially supported by the Minnesota Supercomputing Institute, University of Minnesota.

JEROME, Joseph W (Northwestern University, USA)

Ion transport and gating for channels in cell membranes

Charge transport in channels may be modeled by self-consistent hydrodynamic or Poisson-Nernst-Planck systems. In this talk, principal phenomena will be discussed, such as gating. This has been verified experimentally by means of the patch clamp, and a corroborating mathematical model has been developed in conjunction with Carl Gardner and Robert Eisenberg. If time permits, some connections to action potential propagation will be made.

LUNDSTROM, Mark S (Purdue University, Indiana, USA)

Electron transport in ultrasmall transistors: Physics, issues and approaches

The critical dimensions of transistors are now measured in nanometers, and during the next decade or two, they will shrink to the atomic scale. To explore and optimize new transistors, researchers rely on simulations of charge carrier transport under the influence of their self-consistent electric field. To date, the most used approaches have been based on macroscopic flow equations (so-called drift-diffusion or hydrodynamic-like approaches) or particle simulation by Monte Carlo techniques. As transistor dimensions shrink below 100 nm, new physical effects such as quantum confinement, near collision-free transport, and stochastic effects from the discrete nature of the charge carriers and silicon lattice, are coming into play. My objective in this talk is to present an overview of the transport physics that will have to be captured in future simulations and to identify the transport physics, numerical, and computational issues as seen from the perspective of a semiconductor researcher.

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MSP-075

GARCKE, Harald (Institut für Angewandte Mathematik, Universität Bonn, Germany)

Diffusion in multi phase systems: A phase field approach

We present a phase field concept for interface motion in general multi phase systems with anisotropic interfacial energy. The anisotropy is allowed to be even crystalline which leads to polygonal Wulff shapes. A sharp interface model which appears as the limit of small interfacial thickness is stated. Through a series of numerical simulations we demonstrate that our concept can recover features like crystalline curvature flow, an anisotropic version of Young's law at triple junctions and an anisotropic modification of the right angle condition at points where the interface intersects an external boundary. Finally, we propose a class of potentials with good calibration properties, i.e., potentials whose parameters can be easily adjusted to model prescribed energies and mobilities. As one application, we show that our approach can be used to model the evolution of triple junctions with different symmetries as they occur in certain aluminium systems.

LOGAK, Elisabeth (Universite de Cergy-Pontoise, France)

Analytical derivation of interface dynamics in biological models

We consider a reaction-diffusion system which is derived from a three-component system proposed by M. Mimura as a model with one activator and two inhibitors. When the diffusion of one inhibitor is very large, its concentration is uniform in space and its time evolution is given by an ODE involving the total concentration of the activator. We study the limit free boundary problem and we prove convergence of the solutions of the reaction-diffusion system to the solutions of the free boundary problem, locally in time. This is a joint work with N Bubner, P Laurencot and M Mimura.

NISHIURA, Yasumasa (Research Inst. for Electronic Sci., Hokkaido University, Japan)

Self-replicating dynamics - splitting of interfaces

Self-replicating pattern (SRP) is one of the most exciting dynamics arising in chemical reaction. A localized pattern splits into two parts and continue this process until the whole domain is filled with these completely. The real transient nature of SRP makes the analysis difficult, in fact it does not fall into the usual category of dynamical system theory. We first present a hidden driving mechanism of SRP from a global bifurcation point of view and then discuss why such a structure appears naturally for a class of reaction diffusion systems including the Gray-Scott model. Secondly from an interfacial point of view, self-replication is a typical example of splitting of interfaces. As is known, SRP does not occur when an appropriate parameter is changed, therefore it is quite interesting to study the boundary zone between splitting and non-splitting areas to get an insight of the mechanism of splitting of interfaces.

PAOLINI, Maurizio (Università Cattolica del Sacro Cuore di Brescia, Italy)

Allen-Cahn approximation to crystalline curvature flow

Evolution by crystalline mean curvature is an extreme case of anisotropic mean curvature flow, in which polygonal/polyhedral shapes (like snowflakes) naturally develop during the evolution. It seems to be important in modelling many physical phenomena in which strong anisotropy of the material is present together with surface tension effects at micro/meso-scopic scale. Strange phenomena such as *face stepping* may however appear when dealing with the 3D case. Approximation with a *diffused interface* model such as an Allen-Cahn type bistable reaction-diffusion equation seems to be adequate in naturally reproducing such effects. Moreover such equation is suitable for a numerical discretization. We present known convergence results and some numerical simulations.

RODRIGUES, José-Francisco (CMAF, University of Lisbon, Portugal)

Diffusion free boundary problems: A classical approach

An important class of free boundary problems of Stefan type can be shown to be well posed in a classical sense, at least locally in time, under suitable smoothness assumptions. The approach of Hanzawa has been simplified recently in the light of new uniform estimates in spaces of Holder continuous functions for the respective linearized parabolic systems with time derivatives in the oblique boundary conditions. Those estimates play a central role in the invertibility of the Frechet derivative of an appropriate nonlinear operator. New results, such as the convergence of a Stefan problem to a free boundary combustion problem or the continuous dependence of a superconductivity model with a small kinetic term on the evolving interface, can be obtained when certain parameters with physical meaning vanish. This is a joint work with V A Solonnikov and F Yi.

FUJIMA, Shoichi (Ibaraki University, Japan)

A domain decomposition finite element scheme for flow problems

For computation of flow problems with parallel computers, a domain decomposition finite element scheme for the incompressible Navier-Stokes equations has been proposed by the author. The scheme uses subdomain-wise iso-P2 P1/P1 finite elements for the velocity and the pressure, respectively. In order to connect the velocity among the subdomains, a Lagrange multiplier is introduced and it is discretized by the P1 element. In this talk, algorithm and implementation, especially, data representation technique in distributed memory environment, are discussed to aim at potential of the scheme on super-scalable parallel efficiency. Some applications for CFD problems are also presented.

HANADA, Takao (Chiba Institute of Technology, Chiba, Japan)

Numerical computation of Eguchi-Oki-Matsumura model

Phase separations in binary alloys are interesting phenomena. As the first model, the famous Cahn-Hilliard equation is derived to analyze the spinodal decomposition based on the new free energy. Another model consists of the concentration and the degree of order is introduced by T Eguchi, K Oki, S Matsumura. The well posedness of the system based on this model has been analyzed by the co-author, Masaaki Nakamura. We shall report the occurrence of phase separations from the uniform concentration in numerical computations using this model.

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IKEDA, Tsutomu (Ryukoku University, Japan)

Numerical reproduction of the hexagonal convection pattern

The present talk numerically studies pattern formation in the Boussinesq Rayleigh-Bénard convection problem. The system is a shallow liquid layer heated from the below, and its mathematical model consists of the Navier-Stokes, the continuity and the heat conduction equations under the Boussinesq approximation. Typical experimental example is an excitingly beautiful hexagonal convection pattern, and the purpose of our study is to reproduce this pattern by numerically solving the above mathematical model. We will show both up-hexagonal and down-hexagonal patterns, and report the condition where the hexagonal pattern is selected among others.

This is a joint work with Tadanobu Kimura, Ryukoku University.

ISHIWATA, Tetsuya (Ryukoku University, Shiga, JAPAN)

Analysis and numerical computation for blowing-up solutions arising in a model of curvature flow

Initial-boundary value problems to nonlinear parabolic equation, which are arising in a model of curvature flow, are taken into consideration. The problems have finite time blowing-up solutions. This means that the curvature diverges to infinity in a finite time. Our aim is to analysis the behavior of blowing-up solutions, specially, blow-up rate, blow-up set and asymptotic shape of solution near the blow-up time. First, we present analytical results for special cases. Next, we introduce a numerical scheme discretised by a finite difference method using variable time increment with suitable control and show the numerical results.

NAKAKI, Tatsuyuki (Hiroshima University, Hiroshima, Japan)

Computation to some vortices in the two-dimensional Euler flow

The motion of assembly of point vortices in the two-dimensional Euler flow is a classical problem, which is treated in some detail in textbooks on fluid mechanics. Let us focus our attention on certain special cases of five point vortices. By numerical simulations, we found an interesting phenomenon, that is, a corotating motion with relaxation oscillation. The purpose of this talk is to analyze such a phenomenon from computational and mathematical points of view. It is also shown periodic and chaotic motions of the vortices as well as the motion of finite vortices.

NAKANE, Kazuaki (Osaka Institute of Technology, Osaka, Japan)

A sufficient condition for the existence of global solutions of a one-dimensional hyperbolic free boundary problem

A thin film is pasted on the plate. By lifting up the edge of the film in a vertical direction, we peel off it from a plate." We call this problem "peeling-off". We are interested in the behavior of the film, especially, the motion of the peeling front. The differential equation which describes the motion of film includes the Dirac-delta function, which makes this problem difficult to analyze in mathematically.

We first try numerical computations to this problem and obtain rigorous mathematical results concerned with the global existence of peeling front.

OHMORI, Katsushi (Toyama University, Japan)

Finite element approximation of two-fluid flows including surface tension effect

In this study we consider the finite element scheme for the incompressible, immiscible viscous two-fluid flows including surface tension effect. In order to sharply capture the interface between two fluids we use the pseudo-density function, which is the solution of the transport equation introducing a double well potential. Surface tension effect is modeled by a volume force and is computed by the finite element approximation of the pseudo-density function.

SAKAJO, Takashi (Department of Mathematics, Nagoya University, Nagoya, Japan)

Numerical computation of three-dimensional vortex sheet with swirl flow

We investigate numerically the evolution of three dimensional cylindrical vortex sheet motion with swirl. The implementaion of vortex method and Draghicescu's fast summation method on a parallel computer achieves a practical and high-speed numerical computation. As a result, we find not only an appearance of spiral structure which is seen in two-dimensional vortex sheet motion but also that of new streamwise roll-up structure. We will report the physical and mathematical meaning of the new structure in the talk.

TOMOEDA, Kenji (Osaka Institute of Technology, Japan)

Numerical free boundary in a porous media equation with strong absorption

A porous media equation with a strong absorption: $u_t = \Delta(u^m) - cu^p$ ($m > 1$, $1 > p > 0$) exhibits a remarkable property. The support becomes multiply connected, even if the initial support is simply connected. These phenomena are caused by the degeneracy on $\{x|u(x) = 0\}$ and the effect of a strong absorption. The interface $\partial\{u = 0\}$ appears, and is called a free boundary. In this talk we present the numerical method realizing such phenomena. In the one dimensional case, we state the sufficient condition under which the support begins to split, and present the interface equation determining the behavior of the interface.

ZHANG, Shao-Liang (University of Tokyo, Japan)

Krylov subspace methods for symmetric indefinite systems of linear equations

Symmetric indefinite systems of linear equations arise very frequently in many important applications, for example from Domain Decomposition methods for partial differential equations. In the present paper, convergence behaviour of some Krylov subspace methods for solving such systems are discussed. This is a joint work with M Mori and M Sugihara.

HICKERNELL, Fred J (Hong Kong Baptist University, China)

Error decay rates for Quasi-Monte Carlo quadrature

The error for Monte Carlo (MC) quadrature using N points is $O(N^{-1/2})$, independent of dimension. For quasi-Monte Carlo (qMC) quadrature the error decays like $O(N^{-1}[\log N]^s)$, where s is the dimension of the integration domain. Because of the powers of $\log N$ the asymptotic result does not indicate whether qMC will be superior to MC for large s . This talk summarizes recent derivations of more precise formulae for qMC quadrature error that can be directly compared to that of MC. We see that qMC may still be superior to MC even when s is high.

NIEDERREITER, Harald (Austrian Academy of Sciences, Austria)

Constructions of quasirandom points

Quasirandom points are the deterministic sample points that form the basis of a quasi-Monte Carlo method. The efficiency of a quasi-Monte Carlo method depends in a crucial way on how small the discrepancy of these points is. We report on the state-of-the-art in the construction of quasirandom points, with an emphasis on recent progress.

PAPAGEORGIU, Anargyros (Columbia University, USA)

Quasi-Monte Carlo for problems in mathematical finance

Often problems in mathematical finance require the approximation of very high dimensional integrals. Typical dimensions range from a few hundred to the low thousand. Examples include pricing of financial derivatives and Value at Risk calculations. Our tests for a variety of these problems show that quasi-Monte Carlo is consistently faster than Monte Carlo by one to three orders of magnitude depending on the required accuracy. We discuss our findings and possible explanations for the success of quasi-Monte Carlo.

SLOAN, Ian H (University of New South Wales, Australia)

On the tractability of Quasi-Monte Carlo integration

Integration over the s -dimensional cube has been shown (in recent joint work with H. Wozniakowski) to be intractable in a variety of settings - i.e. the cost of obtaining a guaranteed worst-case error bound less than a fixed number ϵ rises faster than any polynomial as s increases. How, then, can it be understood that in some applications (especially in mathematical finance) researchers claim to be able to evaluate integrals in hundreds of dimensions? In recent work we have shown that quasi-Monte Carlo calculations can indeed be valid for problems in arbitrarily many dimensions, provided that we work in suitably weighted function spaces.

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BERNTSEN, Svend (Aalborg University, Denmark)

Integral equations of inverse scattering of acoustic and electromagnetic waves

The general three dimensional inverse problem of acoustic or electromagnetic waves is formulated by integral equations for the field in the time domain and the refractive index. Using Fourier like transforms the "Born approximation" integral equations are solved analytically. The integral equations are Volterra like, and the permittivity may be reconstructed successively, starting from the boundary of the scatterer. The boundary data in a time interval $[0, T]$ will give the reconstruction of the permittivity in a set Ω for which the reflected wave from Ω has arrived at the boundary of the scatterer in the time interval $[0, T]$. Numerical results will be presented.

FISHMAN, Louis (Naval Research Laboratory, USA)

The role of operator symbols in classical elliptic wave propagation

The n -dimensional, elliptic, two-way Helmholtz wave propagation problem can be exactly reformulated in a well-posed manner as a one-way wave propagation problem in terms of appropriate Dirichlet-to-Neumann (DtN) operators. These operators are formally defined and constructed in an appropriate pseudodifferential operator calculus in terms of their corresponding operator symbols. The analysis and computation of both direct and inverse wave propagation problems can then be largely reduced to the understanding and exploitation of the operator symbol (singularity) structure and the subsequent construction of uniform (over phase space) asymptotic operator symbol approximations. Examples from both direct and inverse scattering will be given.

GUSTAFSSON, Mats (Dept. of Electromagnetic Theory, LTH, Sweden)

Generalised Bremmer series with application to direct and inverse scattering

The generalised Bremmer series consists of a directional decomposition of the wave field and a series of one-way propagation problems. For the direct scattering problem, it offers an efficient numerical algorithm. The Bremmer series is also useful in the inverse problem, where it gives an asymptotic inversion procedure. We discuss the convergence properties of the Bremmer series and illustrate its use in the direct and inverse scattering problems with numerical examples from exploration seismology. This is a joint project with Maarten V de Hoop, CWP, Colorado School of Mines, USA.

JONSSON, B Lars G (Division of Electromagnetic Theory (TET), Royal Institute of Technology, Sweden)

Spectral decomposition of wave splitting in the presence of anisotropy

The method of directional wave field decomposition is a tool for analyzing and computing the propagation of waves. The method is beneficial because it leads to computationally efficient *modeling* algorithms. It can also be used to separate different propagation phenomena, which is of importance in the interpretation and *inversion* of wave-field measurements on a boundary. The extension of directional wave field decomposition to heterogeneous anisotropic media is the subject of this paper. It requires the development of a spectral decomposition of the operator. The decomposition is represented by a projection. This is a joint work with M V de Hoop, CWP, Colorado School of Mines.

KARLSSON, Anders (Department of Electromagnetic Theory, Lund Institute of Technology, Sweden)

Wave splitting and wave propagators in spherical coordinates

A method for decomposing waves in spherical coordinates is presented. The method is based upon an expansion of the electric field in vector spherical harmonics. The expansion coefficients are then dependent on the radial coordinate. From the Maxwell equations a system of ordinary differential equations are derived for these expansion coefficients. These equations are well suited for numerical implementation. Numerical examples will be presented both with a source inside an inhomogeneous spherical shell and for a plane wave that is scattered from an inhomogeneous region. The inverse problem is also discussed.

KREIDER, Kevin L (University of Akron, USA)

Scattering problems for nonlinear viscoelastic rods via wave splitting

A class of nonlinear rods, which includes spatial inhomogeneities, varying cross sectional area and arbitrary memory function, is considered. The wave splitting technique is applied to provide a formulation suitable for numerical computation of direct and inverse scattering problems. Due to the nonlinearity of the material, there are no well defined characteristics other than the leading edge, so the method of characteristics, highly successful in the computation of linear wave splitting problems, is abandoned. A standard finite difference scheme is employed for the direct problem, and a shooting method is introduced for the inverse problem. The feasibility of the inverse algorithm is presented by several numerical examples.

KRISTENSSON, Gerhard (Dept of Electromagnetic Theory, Lund University, Sweden)

Homogenization of woven materials

The effective electric and magnetic material properties of a complex (two-component) mixture are addressed. The mixture is periodic in two directions and has a finite thickness in the third direction. The homogenization problem is solved by a series expansion (multiple-scale technique), and the numerical solution of the two-dimensional vector-valued problem is found by a FEM formulation. The FEM problem is non-standard due to the periodic boundary conditions of the problem. Several numerical computations show that the most important parameter of the effective permittivity is the volume fraction of the guest material in the host, and that the medium in general is anisotropic.

LU, Ya Yan (City University of Hong Kong, Hong Kong, China)

One-way computational techniques for Helmholtz waveguides

For large scale wave propagation problems, it is often necessary to solve a variable coefficient Helmholtz equation in a large domain. Standard numerical methods such as the finite difference and finite element methods lead to very large system of equations, since a few grid points or basis functions are always required to resolve the highly oscillatory wave-field. For waveguide problems, where the length scale is particularly large in the range direction, exact one-way re-formulations of the Helmholtz equation based on Dirichlet-to-Neumann and Neumann-to-Dirichlet maps are particularly useful. Techniques for implementing these one-way re-formulations will be described in this talk. These includes a truncated local eigenfunction expansion for efficient representation of the related operators, large range stepping methods for weakly range dependent waveguides, an automatic switch between different re-formulations to avoid singularities, a local orthogonal transformation for curved boundaries, etc.

OLSSON, Peter (Department of Mechanics, Chalmers University of Technology, Sweden)

Mechanical scattering problems for structural elements

The last few years my group at the Dept. of Mechanics at Chalmers has been working on the application of time domain methods to direct and inverse problems scattering problems in structural elements. The possibility of using bending and shearing wave scattering to reconstruct inhomogeneities in beams and plates has been addressed, and in the present talk some of the results are reviewed. The reconstructions involve geometric as well as material properties, and both straight and curved structures are considered. Some basic problems connected to the modelling of wave propagation in plates and beams will also be touched upon, as well as some problems of optimal design with respect to mechanical wave propagation properties.

POWELL, Jeffrey O (Middle Tennessee State University, USA)

Trace formulae for two-parameter reconstruction in 1D inverse scattering

A frequency domain inverse scattering algorithm for a Helmholtz equation with matrix coefficients. Coefficients are constant outside of a slab; inside, they are inhomogeneous in one direction and represent properties of an anisotropic, absorbing medium. Reflection and transmission data, in matrix form, are collected for several wave numbers at each side of the slab from medium responses to normally and obliquely incident plane waves. Systems of Riccati equations for internal reflection and transmission propagate data into the slab; the unknowns - a permittivity and a conductivity - are computed from matrix trace formulae. Numerical reconstructions from simulated data are displayed.

SJÖBERG, Daniel (Department of Electromagnetic Theory, Lund University, Sweden)

Wave decomposition in nonlinear, anisotropic media

A method to decompose an electromagnetic field in a nonlinear, passive, nondispersive and anisotropic material is presented. Using simple wave theory and six-vector formalism, the Maxwell equations are turned into an algebraic eigenvalue problem. The solution of this eigenvalue problem gives four propagating eigenwaves and two non-propagating. The method can be used to study the behaviour of the optical response in dispersive materials, and provide useful algorithms. Some results on the oblique incidence of plane waves on nonlinear, anisotropic materials are presented.

STROM, Staffan E G (Department of Electromagnetic Theory, Royal Institute of Technology, Sweden)

Identification of current sources in a bounded domain for Maxwell's equations

The inverse problem of determining the spatial current source distribution in a conducting object is formulated, with an emphasis on the case of a current dipole source. Some explicit formulas for identification of the location and moment of the dipole source are derived. The static case is considered, as well as the general case of an arbitrary frequency. Numerical results are presented. This is joint work with Prof. V.G.Romanov and Prof. S. He.

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HOSKING, Roger J (School of Computer Science, Mathematics & Physics, James Cook University, Townsville, Australia)

Asymptotic evaluation of Fourier integral solutions

This presentation surveys the successful application of asymptotic analysis to the mathematical modelling of the response of a floating flexible plate to a moving load. Both steady state and time-dependent plate deflexions are conveniently represented by multiple Fourier integrals. Asymptotic evaluation of the steady state solutions, when distance from the moving load is the appropriate large parameter, has proven to be remarkably accurate even as close as a few load dimensions from the centre of the moving load. Asymptotic evaluation of various time-dependent solutions, when the time variable is taken to be the large parameter, has produced the essential results which define the evolution of the response - including identification of the critical load speed(s) at which the deflexion strongly peaks.

KAMINSKI, David (University of Lethbridge, Canada)

Hills and valleys at infinity for the steepest descent method

The determination of hills and valleys at infinity for the method of steepest descent is a routine task for integrals of a single complex variable. Less apparent is the approach one should take when dealing with the multivariate method of steepest descent. This talk will show how one can use an autonomous system of differential equations and the behaviours of its solutions to extract the hills and valleys at infinity. The setting for the problem is restricted to polynomial phase functions in the integrand, and the method of analysis is reminiscent of the geometric approach of Poincaré in his study of polynomial vector fields in the plane.

LÓPEZ, José L (Department of Applied Mathematics, University of Zaragoza, Spain)

Uniform asymptotic expansions of Bernoulli and Euler polynomials

Bernoulli and Euler polynomials are considered for large values of the order and the variable. Asymptotic expansions are obtained for $B_n(nz + 1/2)$ and $E_n(nz + 1/2)$ in powers of n^{-1} , with coefficients written in terms of hyperbolic functions of argument $1/2z$. These expansions involve certain combinations of incomplete gamma functions and are uniformly valid for z outside certain disks centered at the imaginary axis. Error bounds are also obtained. The strong accuracy of the expansion let us to obtain approximations of the complex zeros of the Bernoulli and Euler polynomials.

This is a joint work with Nico M Temme.

PARIS, Richard B (Division of Mathematical Sciences, University of Abertay, Dundee, UK)

The asymptotic expansion of Gordeyev's integral

In the study of the propagation of electrostatic waves in a hot magnetised plasma one encounters the function defined by $G_\nu(\omega, \lambda) = \int_0^\infty \exp[i\omega t - \lambda(1 - \cos t) - \frac{1}{2}\nu t^2] dt$, $\text{Re}(\nu) > 0$, known as Gordeyev's integral. The real part of the parameter ω represents the normalised wave frequency and the real parts of the parameters λ and ν are respectively the squares of the perpendicular and parallel components of the normalised wave vector. We discuss the asymptotic structure of this integral for large values of ω and λ as $\nu \rightarrow 0+$. For positive real parameters, the real part of the integral is associated with an exponentially small expansion in which the leading term involves a Jacobian theta function as approximant. This expansion is found to be uniformly valid in the frequency parameter ω through a harmonic. The asymptotic expansions are compared with numerically computed values of $G_\nu(\omega, \lambda)$.

WOOD, Alastair D (Dublin City University, Ireland)

Asymptotically-assisted numerics in MHD stability problems

The role of asymptotic analysis in enhancing the effectiveness of numerical methods and reducing their computational intensity is now well established. We take as an example a complex system of coupled ordinary differential equations which arises in the boundary layer structure about a resonant surface when considering resistive instabilities of a high temperature plasma in cylindrical geometry. This is a singular problem on an infinite interval. We use asymptotic information obtained by dominant balance methods to provide a more realistic boundary condition at a finite endpoint for the numerical method, and compare the results with the zero boundary condition case.

BLACKMORE, Denis (New Jersey Institute of Technology, USA)

Quasi-ergodic flows in automated assembly

A fundamental problem in automated assembly can be formulated mathematically as follows: Let M be a smooth, m -dimensional manifold with boundary embedded in Euclidean n -space \mathbf{R}^n . Let $\varepsilon > 0$ and a point $x \in \partial M$ be specified. Find a path ϕ in M starting at x such that for each $y \in \text{Int } M$, $\phi(t)$ belongs to the ε -ball centered at y for some $t > 0$. A flow Φ_t on M having the property that its positive semi-orbit starting at any point on ∂M has the above property is said to be ε quasi-ergodic. We prove existence theorems for ε quasi-ergodic flows for several types of submanifolds and consider the question of optimality related to shortest path orbits. In addition, we discuss algorithms for implementing our theory.

BOGOLIUBOV, Nickolay N (Dept. of Statistical Mechanics at the Steklov Mathematical Institute of the RAN, Russia)

Hartree-Fock-Bogoliubov approximation for model systems with four-fermion interaction

Based on approximation Hamiltonian method, which gives preference investigate dynamical and thermodynamical properties of models with four-fermion interaction. This method includes standard Bogoliubov's trial (approximating) Hamiltonians method for model with separable interaction with Hartree-Fock approximation based on ideas of self-consistency. It gives possible to construct systems of nonlinear equations with sources. As example we also consider BCS model used in the superconductivity theory.

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NAPORA, Jolanta (Dept. of Applied Mathematics, AGH, Krakow, Poland)

The Moser type representation of integrable Riccati-Abel ordinary differential equations and its Lie-algebraic structure

As is known more than one hundred and fifty years ago J. Liouville posed the problem of describing Riccati equations $dy/dx = y^2 + a(x)y + b(x)$ which are integrable by quadratures. But up to now there exists no effective theory answering the question whether a given Riccati equation is integrable or not. Based on the theory of Lax type integrable dynamical systems eighteen years ago there was made a new attempt to study the Liouville problem. Here we devise a new approach to investigating the integrability by quadratures reducing a given Riccati equation to some equivalent nonlinear evolution equations in partial derivatives with Cauchy-Goursat initial data, and proving further their Lax type integrability. This approach having backgrounds in modern differential-geometric and Lie-algebraic techniques, give rise to a partial solution to the Liouville problem. We prove that the integral solutions submanifold is in general not canonically symplectic on which the corresponding vector fields d/dx and d/dt are completely Liouville integrable Hamiltonian systems, whose solutions parametrize too a class of Riccati-Abel equations integrable by quadratures. Some considerations involving the momentum mapping technique and Marsden-Weinstein reduction theory are made concerning the Lie-algebraic study of the Liouville problem for the Riccati-Abel equation .

PERESTIUK, Mykolay M (Dept. of Mathematics and Mechanics of the Kyiv State University, Kyiv, Ukraine)

Stability of invariant torus for impulsive systems

We study stability of invariant torus for the systems of differential equations under impulsive perturbations. Similar problems arises when somebody studies the performance of different machines or mechanisms which are subjected to mechanical forces of impulsive nature. In the terms of properties of Lyapunov functions and their derivatives, calculated by virtue of the differential equations under consideration, we formulate criteria of stability (asymptotic stability, nonstability) of invariant torus for the impulsive systems. See A.M. Samoilenko and N.A. Perestyuk, *Impulsive differential equations*, World Scientific, Singapore, 1995, and A.M. Samoilenko, *Elements of mathematical theory of multifrequency oscillations*, Moscow, Nauka, 1987 (In Russian).

PRYKARPATSKY, Anatoliy K (AGH, Poland and Dept. of Nonlin. Mathem. Analysis, IAPMM of the NAS, Lviv, Ukraine)

On adiabatic invariants of slowly perturbed completely integrable polynomial Focker type Hamiltonian systems

The report is devoted to the imbedding problem of Lagrangean submanifolds of slowly perturbed polynomial completely integrable Focker type Hamiltonian systems and associated with them adiabatic invariants theory. We investigated the structure of imbedding mappings for some Focker type Hamiltonian systems and applied it to finding adiabatic invariants based on the averaging theory and canonical transform method.

PRYKARPATSKY, Anatoliy K (AGH, Poland and Dept. of Nonlin. Mathem. Analysis, IAPMM of the NAS, Lviv, Ukraine)

On the structure of the Lax type formula to the nonlinear Hamilton-Jacobi equations and some its applications

Based on a differential-geometric structure of the invariant compact submanifold (invariant torus) of a Hamiltonian system in case of its complete integrability via Liouville the method of investigating the deformation of slowly perturbed Hamiltonian systems is developed. The defining differential equations for the embedding of the invariant torus into the phase space is obtained. This makes it possible to obtain by means of methods of canonical transformations and the accelerated convergence the existence conditions of adiabatic invariants. The report is devoted to the imbedding problem of Lagrangean submanifolds of slowly perturbed polynomial completely integrable Focker type Hamiltonian systems and associated with them adiabatic invariants theory. We investigated the structure of imbedding mappings for some Focker type Hamiltonian systems and applied it to finding adiabatic invariants based on the averaging theory and canonical transform method. This report is devoted to a proof of validity of the Lax formula (see Crandall M.G., Oshii H., Lions P.-L., *User's guide to viscosity solutions of second order partial differential equations*, Bulletin AMS, v.27, #1, p.p. 1-67 (1992)) for the solution to a free one particle Hamilton-Jacobi nonlinear partial differential equation with Cauchy data being a semicontinuous from below function. A method of finding the Lax type solution to the Cauchy problem of a one class of nonlinear Hamilton-Jacobi equations, having interesting applications (see Aubin J.-P., *L'analyse nonlineaire et ses motivations economiques*, Masson, Paris, (1984)) in modern mathematical physics and economics, is suggested, based on the theory of finite dimensional dynamical systems and their Lagrangean manifolds (see Maslov V.P., *Asymptotical analysis*, Mosciov, Nauka, (1987) and Arnold V.I., *Mathematical Methods in Classical Mechanics*, Graduate Text in Math., v.60, Springer, NY (1987)).

PRYTULA, Mykola M (Lviv State University, Ukraine)

On nonuniform and nonlocal conservation laws of the KdV-equation

The report is devoted to the description of some nonuniform and nonlocal conservation laws of the KdV-equation, making use of analysing special solutions to the characteristic Lax equation. Based on it and the bi-Hamiltonicity of the KdV equation, a reduced linear first order equation in partial derivatives is obtained, whose characteristics are analysed in detail. Statements describing exactly new hierarchies of nonlocal and nonuniform conservation laws are formulated with proofs.

ROSATO, Anthony D (New Jersey Institute of Technology, USA)

Dynamical features of vibrating beds of granular materials

In industries involved with the handling and processing of granular solids, vibrations are often used to enhance or induce flows. Depending on the level and type of vibrations, a bed of particulates can exhibit a wide range of phenomena, such as heaping, compaction, convection, fluidization, surface waves, and arching. In this talk, we examine flows induced through the imposition of sinusoidal oscillations to the floor of a bed of model particles consisting of elastic, frictional spheres. The system is studied through discrete element computer simulations by investigating the effects of a number of parameters on the developed flows. Comparisons are made with kinetic theory predictions from the literature and with physical experiments to provide insight into observed behavior.

SAMOILENKO, Anatoliy M (Institute of Mathematics of the NAS, Kyiv, Ukraine)

Asymptotic method of investigating m-frequency oscillations systems

We present the asymptotic method of integration of $2n$ -order m -frequency oscillation systems and analyze averaged equations in nonresonance and resonance cases. We also prove the theorem on the preservation of smooth p -dimensional invariant tori under perturbation for arbitrary p (0 less or equal p less or equal n) and indicate the types of decomposable m -frequency oscillation systems.

SAMOYLENKO, Valeriy H (Kyiv Taras Shevchenko University, Ukraine)

Specific effects caused by impulse influences in impulsive systems

Numerous engineering and other practical problems are connected with the investigation of nonlinear dynamical systems with short-time process or under the action of external forces whose duration may be neglected in creating the relevant mathematical models. For examples, the mentioned above problems appear in metallurgy (in controlling temperature in thermal and open-hearth furnaces), in chemical technology, in dynamics of aircrafts, in mathematical economics, in medicine and biology, etc. The investigation of mathematical models of these systems leads to the necessity of the analysis of discontinuous dynamical systems generated by ordinary (or partial) differential equations and additional conditions of impulse influences. In the general case, the conditions of impulse influences transform the original dynamical system into essential nonlinear system and may result in a very complicated behaviour of its trajectories. For example, even in the cases when linear differential equations are used in the corresponding mathematical model, the behaviour of trajectories in a dynamical system generated by the linear differential equations with some conditions of impulse influences can be extremely complicated precisely due to the presence of these conditions and may fundamentally differ from the behaviour of trajectories of the given differential equation without of impulses. We study nonlinear systems generated by linear differential equations with conditions of impulse influences, for which a lot of specific effects caused by impulse influences are demonstrated. In particular, for impulsive systems we prove the result on the co-existence of infinite number of periodic regimes ordered according to Sharkovsky order. This effect caused only by the presence of impulse influences and does not exist for the given differential equations when the conditions of impulse influence are absent. The corresponding examples are presented. The mentioned above results are generalized for the case of nonlinear differential equations.

SAMULYAK, Roman (New Jersey Institute of Technology, USA)

Approximate inertial manifolds for granular flow dynamical systems

The concept of the approximate inertial manifold (AIM) is a link between the strong mathematical theory of inertial manifolds and the applied theory of dynamical systems. The AIM is a finite-dimensional smooth surface in the phase space of a dissipative dynamical system such that all the orbits enter a thin neighborhood of the manifold in some transient time. The concept of AIM allows us to reduce an infinite-dimensional dynamical system to a finite-dimensional one called the inertial form, to establish the localization theorems for global attractors and to develop new approaches to numerical investigation of the long-time dynamics. Two numerical methods for the inertial form calculation are developed using the main idea of the AIM theory, namely that the "higher" order modes in an expansion of a solution can be expressed in terms of the "lower" order ones due to nonlinearity of a dissipative system. The first method implements the spectral technique with the set of Chebyshev polynomials as the basis functions. The second method applies the separation of modes idea to finite-differences. The methods are applied to a dynamical system describing granular flows. Numerical calculations show advantages of the methods with respect to the standard numerical schemes.

SIDORENKO, Yuriy M (Lviv State University, Ukraine)

Binary transformations and exact solutions for multidimensional integrable systems

Let $\varphi = \varphi(x, t)$, $\varphi^* = \varphi^*(x, t) = \varphi^T$ are matrix solutions of the evolution system

$$\alpha\varphi_t = L\varphi, \alpha\varphi_t^* = -L^+\varphi, \alpha \in C, \quad (1)$$

where $L = \sum_{i=0}^n u_i D^i$ is $(N \times N)$ - matrix differential operator with smooth coefficients $u_i(x, t) \in$

$Mat_{N \times N}(C)$, $i = 0, 1, \dots, n$, $L^+ := \sum_{i=0}^n (-1)^i D^i u_i^T$ is transposed operator. The following statements are true.

Theorem 1. Function $\psi\varphi : R^2 \rightarrow Mat_{M \times M}(C)$ is a density of local conservation law for the system (1), i.e., $(\psi\varphi)_t : \frac{\partial}{\partial x} P[u_i, \varphi, \psi]$, $i = 0, 1, \dots, n$, where P is differential polynomial of variables indicated in the parenthesis.

Theorem 2. The system (1) is covariant in respect of transformation of wave function of the following form:

$$\varphi \rightarrow \Phi = \varphi \left(\int^x \psi\varphi dx \right), \psi \rightarrow \Psi = \varphi \left(\int^x \psi\varphi dx \right), \quad (2)$$

i.e., the following equations take place $\alpha\Phi_t = \tilde{L}\Phi, \alpha\Phi_t^* = -\tilde{L}^+\Phi^*$, where $\tilde{L} = \sum_{i=0}^n \tilde{u}_i D^i$, $\Phi^* = \Psi^T$. The transformations (2) is a vector generalization of binary transformations of Darboux type for the case of arbitrary matrix differential equations. The effectiveness of applications of binary transformations (2) is demonstrated for famous (2+1)-dimensional integrable systems of soliton theory. The exact solutions of the systems under consideration are found.

ENGL, Gabriele (Linde AG, Process Engineering and Contracting Division, Germany)

Model identification of a catalytic reactor for alkane dehydration

A typical approach in computer-aided process engineering involves the model development on the basis of pilot plant data in order to simulate and optimize scale-up plants for full-size industrial application. As an example, the catalytic dehydration of alkanes is presented. The simulation model of a catalytic fixed-bed reactor is derived, and model parameters are identified. Control strategies for a large-scale discontinuous production plant are developed and optimized. The computations are performed by the Linde in-house, equation-oriented process simulator OPTISIM[®]. A wide range of mathematical problems is encountered, e.g. the appropriate PDE discretization, solution of discontinuous DAE systems, steady-state and dynamic optimization problems. This is a joint work with Andreas Kröner, Linde AG, Process Engineering and Contracting Division, Höllriegelskreuth, Germany.

MRZIGLOD, Thomas (Bayer AG, Leverkusen, Germany)

Application of neural networks in chemical industry

Artificial neural networks are an efficient mathematical tool for bringing to light knowledge, that is only latently existent in numerous databases or data acquisition systems and harnessing this knowledge to applications. In particular, neural networks make it possible to establish direct models for the quality variables of products (e.g. viscosity, stability, visual properties, etc.) as a function of their composition or of operating parameters. One focal point of applications in chemical industry are the evaluation and optimization of test series for forecasting product properties and for formulation calculation. The other focal point is the use of neural networks for setting up models of processes and plants.

PANTELIDES, Costas C (Imperial College of Science, Technology and Medicine, London, UK)

Some recent developments in the optimisation of hybrid discrete/continuous processes

Most chemical processes of practical interest are hybrid in nature, exhibiting both discrete and continuous characteristics. The discrete aspects arise both from external discrete manipulations imposed on the process and/or from discontinuities that are intrinsic to its physical behaviour. Simulation of even quite complex hybrid processes is now a routine activity. On the other hand, hybrid process optimisation is still in its infancy. We present a mathematical formulation of the optimisation of hybrid processes based on their formal description in terms of state-transition networks. We also briefly review methods for the solution of this type of problem, and present some representative examples.

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SUNDMACHER, Kai (Max-Planck-Institut fuer Dynamik komplexer technischer Systeme, Magdeburg, Germany)

Methods and tools for modelling and simulation of fuel cells

Fuel cells can generate electrical energy for transportation purposes or stationary power supply by electrochemical oxidation of components such as hydrogen, methanol or methane in environmentally friendly processes. One of the most innovative fuel cell concepts is the DMFC (Direct Methanol Fuel Cell). In the cell methanol is oxidized to carbon dioxide at the anode and oxygen is reduced to water at the cathode. To understand the DMFC steady state and dynamic behaviour, there is need for a sound engineering analysis of this complex multi-phase system based on a rigorous mathematical modelling and simulation strategy. In this contribution, first alternative methods and tools for fuel cell modelling and simulation are reviewed and compared. Then, a hierarchical model for the DMFC is presented which combines the mass and charge balances with kinetic expressions for the chemical reactions and the mass transport phenomena. The set of model equations form a differential-algebraic system (DAE) which can be solved by application of the DAE-solver LIMEX. The model is used to simulate the parametric behaviour of the cell and the dynamic response to perturbations of process input variables such as the feed composition.

WAIT, Richard (MidSweden University, Sweden)

Modelling of thermomechanical pulping

Wood Pulping plants that make use of thermomechanical pulping are more friendly to the near environment than those based predominantly on chemical pulping technology. However, mechanical pulping consumes large quantities of potentially very expensive electricity and continual improvements in the design are vital if this form of technology is to remain economically viable. The central part of the process is the refiner where wood chips is defibrillated into fibres. The refiner consists of two circular discs, placed concentrically, one of which rotates (or both rotating in opposite directions). The distance between the discs is of the order of a millimetre. Wood chips enter at the centre and are transported out between the discs by centrifugal forces and defibrillated into fibres by contact with the radial bars on the discs. The chips and the fibres are dispersed in water at the inlet. The water is converted into steam in the refiner by the heat generated by the friction and defibrillation. The performance of the refiner is very sensitive to a number of variables, such as the form of the grinding surface, distance between the discs, inlet consistency of the wood chip - water mixture and throughput. A good mathematical/computational model greatly enhances both the design process and the optimisation and control the production of pulp. The commercial goal of the industrial partners is to design a refiner that produces better quality pulp at a lower price.

The computational models discussed involve a number of coupled, non-linear differential equations with variables such as water-, steam- and fibre-velocities, temperatures, etc. The development of a parallel finite element model used for graphical representation of the chip flow will also be discussed.

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CARRILLO, José A (Department of Mathematics, University of Texas at Austin, Texas, USA)

On some kinetic equations arising in granular media

This talk will be devoted to discuss some properties of the asymptotic behavior of solutions of kinetic equations modeling granular media. Hydroynamical limits and its validity will be discussed. The first part of the talk will be devoted to a 1-D model of a granular material on a thermal bath. The second part will treat some results on the homogeneous solutions of a simplified inelastic Boltzmann equation in 3-D with constant and variable restitution coefficient. We will discuss the validity of the hydrodynamical limit based on this discussion.

CASTELLANOS, Antonio (University of Seville, Seville, Spain)

Mechanical properties of fine powders and its relationship to interparticle forces

The tensile strength and the average free volume for a set of cohesive powders (toners) have been measured as a function of the consolidation stress and void fraction. The experimental technique is fully automated, using direct and reverse flows to initialize, consolidate and break the powders. The measurements indicate that as the consolidation stress increases, the tensile strength changes from a linear to a sublinear function of the consolidation stress. The theory developed by Maugis and Pollock indicates that for low magnitude interparticle forces contact between particles is fully plastic. For larger magnitudes, the contact becomes plastic with elastic recovery.

This is a joint work with J M Valverde and P K Watson.

GREMAUD, Pierre (North Carolina State University, USA)

Numerical simulations of granular flows in hoppers

We consider the problem of a granular material flowing out of a hopper under the action of gravity. In some, but not all, situations, such problems can be modeled by systems of nonlinear hyperbolic conservation laws, having the stress components as unknowns. The corresponding numerical challenges, which include the presence of nonlinear boundary conditions and algebraic constraints, are discussed. The numerical implementation of a high order discontinuous Galerkin method is considered. Numerical results are presented.

This is a joint work with J V Matthews.

HARRIS, David (University of Manchester Institute of Technology, UK)

Industrial and engineering applications of a new model of granular flow and deformation

A novel, plasticity based continuum model comprising equations governing the stress, velocity and density fields in a deforming or flowing granular material is presented. The model has been developed as a solution to the problems that have beset existing models, examples of which are, the incorporation of internal friction and dilatancy as independent parameters, ill-posedness of the governing equations and the occurrence of negative work-rate in sub-regions of the deforming region. The model consists of a set of first order hyperbolic partial differential equations and these are presented in Cartesian, tensorial and characteristic forms. The archetypal industrial and engineering application of the flow of granular material is hopper flow and a generic initial/boundary value problem for such applications is presented. Results for a specific example of hopper flow are also presented.

HAYES, Brian T (Stevens Institute of Technology, USA)

Response of a finite-depth saturated soil to a single-pulse disturbance

We study four initial-boundary value problems in the strip $0 \leq x \leq L$, $t \geq 0$, for a system of equations modelling a saturated granular medium; this system incorporates a hypoplastic constitutive law. In each problem, a single pulse in either stress or velocity is prescribed along $x = 0$, along with either constant stress or constant velocity at $x = L$. We find that the velocity-pulse/constant-velocity solution comes to rest for all parameter values, and derive a formula for the asymptotic stress. In the other three problems, the solutions become time-periodic oscillations for almost all parameter values.

OSINOV, V A (University of Karlsruhe, Germany)

Dynamic problems for granular media based on hypoplasticity

Dynamic equations for granular materials such as sand are fully nonlinear. A classical solution to such a system may exist only for a finite time, if at all. In addition, the locally linearized equations can lose hyperbolicity. All this suggests that we are dealing with an ill-posed problem. The challenge is to elaborate a proper numerical algorithm in order to obtain physically reliable solutions. A series of numerical solutions has been obtained for dry and saturated soils with the use of the hypoplasticity theory. In particular, it is shown that the longitudinal and the transverse components of velocity are coupled and induce each other. A periodic disturbance of a layer of a saturated soil is shown to result in the liquefaction of the soil with a nonuniform pattern.

PITMAN, E Bruce (Department of Mathematics, State University of New York, Buffalo, USA)

Thoughts on a mechanical theory for particle-fluid flow with solids stress

Granular materials, like sand, soil, or powder, may be characterized as a fourth state of matter. These materials can support stresses like a solid, but also can flow like a liquid. The richness and scope of the dynamics of granular materials rivals that of fluid dynamics. For fine powders, the presence of interstitial fluid is important. Although there is a substantial history of research on particle-fluid flows, especially Stokes flow and fluidized beds, less is known about the dynamic behavior of a high solids volume fraction particle-fluid system. This talk will introduce some of the issues that arise in modeling particle-fluid systems. Of particular importance is the role of frictional particle stress in the governing constitutive relations. Strengths and weaknesses of phenomenological "two fluid" models will be discussed. A new proposal for a numerical model of particles moving in a fluid will be introduced.

SHEARER, Michael (North Carolina State University, USA)

Properties of granular materials

In this talk, I will survey some of the mathematical properties of models of granular materials. I will also discuss issues related to the use of these models for industrial applications.

SLEMROD, Marshall (Center for Mathematical Sciences, University of Wisconsin, Madison, USA)

Generalized rational approximation and Chapman Enskog expansion

The classical Chapman Enskog expansions for the pressure deviator P and heat flux q provide a natural bridge between kinetic and continuum descriptions of gas dynamics. Truncation of these expansions beyond first (Navier-Stokes) order yields instability of the rest state and is inconsistent with thermodynamics. This talk shows how an approximate sum of the Chapman-Enskog expansion via generalized rational approximation eliminates the instability paradox and yields gas dynamics consistent with thermodynamics. Applications to granular flow may also be presented.

SPENCER, Anthony J M (University of Nottingham, UK)

A model for granular material mechanics combining double-shearing and critical state concepts

Models for the mechanical behaviour of granular materials have been classified as belonging to one of two types; type I theories are based on Coulomb-like failure criteria and kinematic assumptions for the shearing mechanism. Type II theories employ the critical state concept and use the state boundary surfaces as plastic potentials. Here a hybrid theory is proposed that combines the critical state concept with the physically based double-shearing mechanism, but rejects the use of a plastic potential.

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HOLM, Darryl D (Los Alamos National Laboratory, USA)

The Euler-Poincaré theorem, integrable PDE's and a new closure model for turbulent channel flow

This lecture will discuss: (1) The Euler-Poincaré theorem unifying Hamilton's principles on groups and on their Lie algebras for right-invariant Lagrangians. (2) The 1D integrable Camassa-Holm equation (CHE) and other equations for geodesic motion on the diffeomorphism group, derived in the framework of the Euler-Poincaré theory. (3) How the 3D version of the CHE is derived in this framework, by applying asymptotic expansions, two-timing and averaging in Hamilton's principle for an ideal incompressible fluid. (4) A new closure model for channel turbulence based on a viscous version of the 3D CHE. Comparison with experimental data. (5) Possible applications in ocean and atmosphere dynamics.

LEITH, Cecil E (Isaac Newton Institute, Cambridge, UK)

Shallow water turbulence

Shallow water dynamics is that of a polytropic two-dimensional compressible gas with index $\gamma = 2$. A simulation of shallow water using the numerical scheme of Arakawa and Hsu (1990: Monthly Weather Review 118, 1960-1969), which has many desirable conservation properties, is used to study Reynolds gas dynamics, i.e., the dynamics of a turbulent gas, and, in particular, the interaction of a shock with turbulence.

MAHALOV, Alex M (Arizona State University, USA)

Fast singular oscillating limits of stably stratified three-dimensional Euler-Boussinesq equations

The 3D rotating Boussinesq equations (the "primitive" equations of geophysical fluid flows) are analyzed in the asymptotic limit of strong stable stratification. The resolution of resonances and a non-standard small divisor problem are the basis for error estimates for such fast singular oscillating limits. Existence on infinite time intervals of regular solutions to the viscous 3D "primitive" equations is proven for initial data in H^α , $\alpha \geq 3/4$. Existence on a long time interval T^* of regular solutions to the 3D inviscid equations is proven for initial data in H^α , $\alpha > 5/2$ ($T^* \rightarrow \infty$ as the Froude number $\rightarrow 0$).

MORRISON, Philip J (University of Texas at Austin, USA)

An integral transform for shear flow

The linear dynamics of inviscid shear flow in a channel is solved by means of a novel integral transform. The integral transform, a generalization of the Hilbert transform, maps Rayleigh's equation into an equation that is trivial to solve. Inversion of the transform thus gives the solution. The integral transform provides a means for describing the dynamics of the continuous spectrum, which is a result of the presence of critical layers, without the inclusion of viscosity or nonlinearity. Numerical implementation of the transform provides an effective means of resolving the fine scale structure that develops in the vorticity. The transform is also used to describe the response of the shear flow system with external forcing and general forms of damping. Several examples are given.

TITI, Edriss S (University of California, Irvine, USA)

On the connection between the Camassa-Holm equations and turbulence theory

In this talk we will show the global well-posedness of the three dimensional viscous Camassa-Holm equations. The dimension of their global attractor will be estimated and shown to be comparable with the number of degrees of freedom suggested by classical theory of turbulence. Furthermore, we will show that by using the Camassa-Holm equations as a closure model to the Reynolds averaged equations of the Navier-Stokes one gets very good agreement with empirical and numerical data of turbulent flows in infinite pipes and channels.

CAMPBELL, Stephen L (North Carolina State University, USA)

Numerical DAE integrators and control

There is an established and growing literature on DAE integrators. DAEs arise in a variety of control problems. This talk will address some issues involved in the application of DAE integrators in control problems including the special demands that can be placed on the integrators. Specific types of control problems will be discussed.

KUNKEL, Peter (Univ. Oldenburg, Oldenburg Germany)

Numerical solution of over and underdetermined differential algebraic equations

Differential algebraic systems with nonunique solutions arise in many application areas. The nonuniqueness may for example arise from the presence of control variables or since the model cannot be completely specified. Most current numerical methods, however, can only deal with uniquely solvable systems. We present some recent progress in the analysis of over- and underdetermined differential algebraic systems and their numerical solution. This is a joint work with P Kunkel, Univ. Oldenburg.

SIMEON, Bernd (FB Mathematik, TU Darmstadt, Germany)

Weak descriptor forms for constrained motion in elastodynamics

Constrained mechanical systems including both rigid and elastic bodies are a focus of current research in computational mechanics and meet the increasing demand for refined simulation in vehicle dynamics, robotics, and in air- and spacecrafts. While rigid bodies form discrete systems in space and are easily modelled by differential-algebraic equations, their elastic counterparts satisfy the partial differential equations of elastodynamics. Mutual coupling is accomplished by constraints formulated for isolated spatial points or parts of the boundary or some subdomain. The talk presents a general framework for the treatment of constraints in elastodynamics and introduces the notion of a *weak descriptor form* which comprises both rigid body systems and mixed systems and which can be considered as a descriptor form model in both space and time. With respect to space discretization, there is a direct connection to mixed and hybrid finite element methods and to domain decomposition techniques.

STÖVER, Ronald (Zentrum für Technomathematik, Universität Bremen, Germany)

A new collocation method for solving linear differential-algebraic BVP

We consider BVP for linear differential-algebraic equations with variable coefficients of the type $E(t)\dot{x}(t) = A(t)x(t) + f(t)$, $Cx(a) + Dx(b) = r$ without any restriction for the index of (E, A) . A well known regularization procedure yields an equivalent index-1 problem with d differential and $a = n - d$ algebraic equations. The collocation method is based on this regularized BVP and approximates the solution x by a continuous piecewise polynomial of degree k and delivers, in particular, consistent approximations at meshpoints by using the Radau scheme. Under soft assumptions the collocation problem is uniquely and stable solvable and, if the unique solution x is sufficiently smooth, convergence of order $\min\{k + 1, 2k - 1\}$ and superconvergence at meshpoints of order $2k - 1$ can be shown.

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ALIEV, Baymurod (Tajik State National University)

Linear ill-posed problems in spectrum

The following problem is typical: let us find a solution in spectrum of the second kind operator equation with a linear compact operator, acting from Hilbert space H to Banach space B , where B is a subspace of H . We suggest that the operator and the right are given approximately. We consider three methods of stable approximation of the unknown normal solution of the equation. The methods are based on Tikhonov regularization and iterative methods, including methods with Chebyshev's parameters. Their properties are investigated. The integral equation of Fredholm of the second kind is taken as an example.

ISKENDEROV, Asaf Dashdamir (Dept. of Optimization and Control, Baku State University, Azerbaijan)

Iterative regularization of the problem about determination of the memory kernel

In the report the nonlinear Abel integral equation in L_p spaces is considered. We derive stability estimates in exponentially weighted L_p -norms and discuss their consequences for iterative regularization of considering problem. Also we established the theorems of existence and uniqueness of solution.

KISS, Eva Maria (Department of Materials Sciences, Freiberg University of Mining and Technology, Germany)

Identification of memory kernels in viscoelasticity - a comparison of three regularization techniques with discretization and numerical examples

We deal with the inverse problem of identifying memory kernels in viscoelasticity under the additional knowledge of the displacement in an interior point of the considered space interval. Three different regularization methods have been successfully applied to solve this ill-posed problem.

The first method consists in a constrained discretized least-squares approach, based on the restriction of the class of admissible kernels to a compact subset of $H^1(0, T)$. Another method is to replace the original problem by a well-posed nonlinear one: a convolution equation of second kind, and an ill-posed linear one: numerical computation of the third derivative. As third method we studied Tikhonov regularization directly on the nonlinear problem.

This is a joint work with L v Wolfersdorf and J Janno.

KURAMSHINA, Gulnara (Faculty of Chemistry, Moscow State University, Moscow, Russia)

Inverse problems of vibrational spectroscopy

New numerical methods for solution of inverse problems of molecular spectroscopy are considered. These problems are connected with a finding the molecular equilibrium geometry and force field parameters from the experimental data (obtained by means of electron diffraction and vibrational spectroscopy methods) and results of quantum mechanical calculations. Numerical algorithms are based on the theory of regularization of nonlinear ill-posed problems.

References: I.V.Kochikov, G.M.Kuramshina, Yu.A.Pentin, and A.G.Yagola. Inverse problems of vibrational spectroscopy. - Moscow, Moscow State University Publ., 1993; Zeist, VSP Scientific Publ., to be published in 1998.

YAGOLA, Anatoly (Faculty of Physics, Moscow State University, Moscow, Russia)

Ill-posed problems and a priori information

We shall consider ill-posed problems with a priori information of the following types: 1) unknown solution is monotonic (or convex, etc.) function; 2) unknown solution is sourcewise represented. We shall discuss the question how to use a priori calculated approximation for construction of unknown solution of ill-posed problem. We would like also to discuss some fundamental concepts and results of the theory of ill-posed problems. In application we shall describe some ill-posed problems in astrophysics and vibrational spectroscopy.

References: 1. A.N.Tikhonov, A.V.Goncharsky, V.V.Stepanov, and A.G.Yagola. Numerical methods for the solution of ill-posed problems. - Dordrecht, Kluwer Academic Press, 1995. 2. A.N.Tikhonov, A.S.Leonov, and A.G.Yagola. Nonlinear ill-posed problems. - London, Chapman and Hall, 1998. 3. I.V.Kochikov, G.M.Kuramshina, Yu.A.Pentin, and A.G.Yagola. Inverse problems of vibrational spectroscopy. - Moscow, Moscow State University Publ., 1993; Zeist, VSP Scientific Publ., to be published in 1998.

GILLIGAN, Christopher A (University of Cambridge, UK)

Modelling dynamics of fungal diseases in plant populations: scaling up from fungal colonies to regions

We describe recent work which emphasises parsimony and model reduction and the analysis of transients including the consequences of interrupted transients for dynamically generated variability amongst replicate epidemics to model the spread of disease through plant populations at a range of scales from microscopic interactions amongst hyphae within fungal colonies to disease patches in fields and to the regional invasion and control of introduced diseases such as Dutch elm disease and rhizomania.

The talk arises from joint work in the Botanical Epidemiology and Modelling Group at Cambridge, involving theoreticians and experimenters, Adam Kleczkowski, Doug Bailey, Wilfred Otten, Adrian Stacey, James Truscott, Jonathan Swinton, Andrew Park and Simon Gubbins, and collaborative work with Gavin Gibson at BioSS, Edinburgh

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HAMBLY, Ben M (University of Edinburgh, UK)

Martingales in the study of the contact distribution in plant epidemics

This talk will consider the estimation of the contact distribution in some simple models for plant epidemics. We assume that new disease sites are dispersed from existing sites according to a spatially symmetric contact distribution and derive estimators for key unknown parameters of this distribution, such as the variance and fourth moment, via martingales. Using martingale central limit theorems it is possible to show the asymptotic normality of these estimators. This suggests how to recover information about the contact distribution from the large scale disease patterns.

MARION, Glenn (University of Strathclyde, Glasgow, UK)

Scaling behaviour in spatial-temporal models for two species reactions

We study a reaction diffusion process with two initially separated reagents, only one of which is mobile. This can be regarded as a simple description of aerobic deterioration (e.g. in silage). The model is formulated as a spatially discrete Markov process. A diffusion approximation is obtained by taking a continuous limit of a mean-field like approximation to the stochastic process. Scaling exponents which characterise the width and height of the reaction front at large times are obtained from these reaction-diffusion equations. However, in the 1-dimensional case these exponents are at odds with those obtained from the stochastic model.

SHERRATT, Jonathan A (Dept of Mathematics, Heriot-Watt University, Edinburgh, UK)

Microscopic vs macroscopic mathematical models for spatiotemporal dynamics during wound healing

The interaction between cells and their environment is the central ingredient of the wound healing process. It results in a coordinated spatiotemporal response to injury, with a large number of cells entering the wound from surrounding tissue to induce repair. A variety of continuum (macroscopic) mathematical models have been developed in the last decade, to study various aspects of the repair process. Although these models have been successfully applied, their formulation prevents them being used to study phenomena that depend on the intrinsic cellularity of the tissue. Recently, several models have been proposed that deal with the microscopic details of the tissue. I will discuss both approaches and compare their predictive capabilities for the development of new clinical therapies.

VAN DEN BOSCH, Frank (Wageningen Agricultural University, The Netherlands)

Pattern formation in spider mite - predatory mite systems

Spider mites form small sedentary colonies on plant leaves. From these colonies individuals disperse through the air. After landing elsewhere they form new colonies. Spider mite colonies can be invaded and destroyed by predatory mites. Predatory mites disperse from destroyed colonies through the air and can invade new spider mite colonies. The system of sedentary colonies and spatially dispersing individuals is modelled. The model is analyzed both analytically and numerically. It is shown that the spatially homogeneous steady-state loses stability through a Hopf-bifurcation. Numerical solutions elucidate the dynamic patterns present in this system. This is a joint work with M de Gee, Mathematical Methods and Models, Agricultural University of Wageningen, Dreijenlaan 4, 6703 HA Wageningen, the Netherlands.

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BODE, Joerg (BMW Rolls-Royce Aero Engines GmbH, Germany)

Design of a thermo-stable satellite antenna

The presentation shows the advanced composite design of an in space polarization sensitive reflector for the DFH3 satellite. The approach uses special optimization techniques and the FE-method including transverse shear stiffness for a twin parabolic shell out of kevlar-nomex sandwich. The requirement of high temperature gradients and big differences in "the day and night" configuration in orbit lead to a character definition of the shell. The special character is defined with the help of a weight function, mostly combining the character of focal point constantness with low weight. Different layouts for shells with good "character functions" are presented with the link made to the metric of the shell. This leads to a layout philosophy, where the metric and curvature characters of shells in composite guide the ply layups of the final design. With the knowledge of Gauss curvature and medial curvature values of the shell a judgement on the E1/E2 and CTE1/CTE2 relationship can be made. All shells of this kind are low in weight and have a constant focal point reflection characteristic for high temperature loads.

LENK, Olaf (Technical University of Berlin, Berlin, Germany)

Weight optimized layout of a high pressure compressor core fairing of a turbo engine

The presentation will give a clear description of a composite layout of a compressor fairing on a BR715 turbo engine with respect to high temperature and pressure loads. Within the design FE-Optimization and engineering judgement was taken as an aid to come to a low weight solution with stiffness control and endurance stress requirement. The high endurance life is coupled with a certain allowed stiffness threshold to avoid aero flutter effects, which can be proven by using equivalent stiffness checks during the optimization runs. After the development of different proposals for a low weight fairing, the link between the metric of the shell and the re-enforcement ply layup is shown. With the same analogy as it was used in the first lecture by J. Bode the curvature values of the shell are taken as master parameter to find the stiffness definition for the shell. The stiffness definition for a good shell with high endurance life as a final target is given for meridian and axial re-enforcement as well as for the CTEs. With this knowledge a family of low weight shells can be designed using just the geometry of the shell one like to have. The geometry lead to the ply layup by taking a special character function, whereas the character function is compiled out of the wished tasks for the shell.

MIDDENDORF, Peter (University of the Federal Armed Forces, Munich, Germany)

Structural layout of the Lunarstar subsatellite GAUSS using a CFRP-sandwich design

The structural design of GAUSS is determined by severe mass and volume constraints (16.5kg total mass, maximum diameter 450mm). In order to keep the structural mass to a minimum and to guarantee the necessary structural strength and stiffness, the load carrying structure, which is a central tube mounted on an upper and a lower base plate, will be built of CFRP-sandwich plates only. The FEM-analysis with MSC/NASTRAN proofs the feasibility of the design and shows some possibilities to optimize the composite layout for a varying spectrum of quasistatic, dynamic and acoustic loads, depending on equipment and launcher rocket.

SCHURIG, Michael (BMW Rolls-Royce Aero Engines GmbH, Germany)

Flaw tolerant design of load carrying composite shell structures

In the presentation a flaw tolerant design concept is proposed for large shell structures out of carbon fibre re-enforced plastics. The example is given on the structural bypass duct of the 14,000 lbs thrust BR710 turbo engine, which is a cylindrical composite shell using sandwich design methods. The flaw tolerant design is situated in between the safe life and the damage tolerant layout, allowing for initial flaws and defects on the structure with no impact to the promised life. In terms of lifing philosophy the flaw tolerant approach classifies special defects and local impact damages with the requirement of ensuring fatigue loads and limit loads during the life period of the engine. To achieve this target, composite crack propagation analyses were performed to assess the residual life once a crack occurs which is a usefull additon to the current safe life approach. It can be shown, that a flaw tolerant design has the potential to be as well imperfection tolerant for buckling load cases, so that the safe life condition is extended by a group of defects, which can be allowed without hazarding the safety of the entire part. For this analyses the extended lamiate theory was used and in addition to that transverse shear delamination was taken into account to follow up in detail the history of crack development in the ply layups.

ANDERSSON, Börje B A (The Aeronautical Research Institute of Sweden)

Mathematical models for damage growth in composite materials

Structural degradation of composite structures, i.e. fiber and matrix cracking, delamination buckling etc is characterised by crack formation on several length scales with partly strong interaction. Due to the variability in material data and production techniques, numerical methods must also consider statistical aspects. In the lecture, mathematical models used to analyse this problem are reviewed. We focus on multi-scale damage problems with multiple-crack growth where statistical approaches are mandatory. Numerical solutions, derived with novel computational procedures, to challenging problems, are presented and numerical results compared with data from laboratory testing.

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CHARALAMBIDES, Panos G (University of Maryland, Baltimore County, USA)

A modified p-method finite element developed for the study of woven composites

Woven composites have complex three-dimensional geometries and intricate microstructures, which makes classical three-dimensional finite elements too computationally intensive to be practical in capturing their non-linear damage response. We present a p/spectral finite element method for general composite systems exhibiting periodic microstructure. Our technique utilizes a semi-analytical method in which the stiffness matrix over each periodic cell is constructed via trigonometric polynomials whose degree can be increased to achieve accuracy. The global response is then recursively updated. The element efficiency is demonstrated with the aid of the compact tension mode I fracture specimen. This is a joint work with S-I Haan, P G Charalambides and M Suri.

MATACHE, Ana-Maria (Seminar for Applied Mathematics, ETH Zurich, Switzerland)

Generalized p - finite elements in homogenization

We propose and analyze a new p - version FEM for elliptic problems with locally periodic microstructure. A class of microscale adapted shape functions is constructed by sampling a generalized Green function in Fourier space and a well conditioned hierarchic system of FE shape functions is then provided by orthogonalizing the coefficient matrix of the unit - cell FE solutions at the sampling points. This yields a generalized p - FEM with robust exponential convergence with respect to the microscale ϵ for piecewise analytic input data.

BLATOV, Igor A (Voronezh State University, Russia)

The Galerkin finite element method for singularly perturbed elliptic and parabolic equations

In this report the Galerkin finite element method for one- and two- dimensional linear and quasi-linear singularly perturbed elliptic and parabolic equations are considered. The finite-dimensional spaces, test and trial, are constructed on the adaptive to boundary layer meshes with M gridpoints, where M is independent from small parameter. For two-dimensional problems the test and trial functions are piecewise-linear in interior domain and piecewise-bilinear in boundary layer. We prove existence of the solution of the Galerkin problems and the second order error estimates.

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NEFEDOV, Nikolai (Department of Mathematics, Faculty of Physics, Lomonosov Moscow State University, Russia)

Singularly perturbed systems in the case of exchange of stability

We consider singularly perturbed systems assuming that reduced problems have intersecting solutions such that standard theory cannot be applied. We introduce the conception of composed stable solution and by means of differential inequalities technique we prove the existence, local uniqueness and asymptotic stability of these solutions as solutions of corresponding parabolic problems. Results can be applied to some chemical problems.

NIKITIN, Andrey G (Department of Mathematics, Faculty of Physics, Moscow State University, Russia)

The solutions with internal and boundary layers of singularly perturbed boundary value problem for integro-differential equations

The boundary value problems for nonlinear ordinary singularly perturbed integro-differential equations are considered. The asymptotic expansions of solutions with internal and boundary layers are constructed. The asymptotics are proved by asymptotic differential inequalities method.

SHARUDA, Dmitry V (Voronezh State University, Russia)

Asymptotical expansion of Cauchy problems for singularly perturbed delay systems

The Cauchy problem for linear singularly perturbed systems of differential equations with the delay are considered. In order to find the asymptotical expansion of the solution a modified method of boundary layer functions is suggested. The principal idea of the method is introducing sequence of fast scaled time variables delayed relatively one another. So the i -th approximation contains the boundary layer functions depending on i fast variables. The algorithm of finding terms of the expansion is constructed. Uniform estimates with respect to "t" of the approximation error are established. Due to the constructed asymptotical expansion the derivatives of the solution are estimated.

STRYGIN, Vadim V (Voronezh State University, Russia)

Vibrational control of singularly perturbed delay systems

It is known vibrational control technique was presented by S M Meerkov and consist in introduction of such vibrations (with mean value equaled zero) of the dynamic system parameters, which modify the properties of the system in a desired manner. Vibrational control has found several important applications, such as stabilization of particle beams, plasmas, lasers and chemical reactors. In this talk a new class of singularly perturbed control systems is considered. To investigate these systems we propose to use hybrid asymptotical method, based on averaging algorithm and boundary layers functions method by A B Vasil'eva.

VASILIEVA, Adelaida B (Department of Mathematics, Faculty of Physics, Moscow State University, Russia)

Contrast structures of alternating type

The singularly perturbed parabolic problem is considered. The periodic with respect to t solution which is equal to zero at the boundary points $x=0$, $x=1$ is investigated. Under some conditions this solution may change his form from the solution having an interior layer of step type to the solution of pure boundary layer type. The asymptotic analysis of such solution is developed. The theory is illustrated by numerical results for some example.

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AFTALION, Amandine (DMI Ecole Normale Supérieure, France)

On the solutions of the one dimensional Ginzburg-Landau equations for superconductivity

When a superconducting film of constant thickness (between the planes $x = -a$ and $x = a$) is submitted to an exterior magnetic field h_0 , the state of the sample can be described by the functions $f(x)$ and

$$q(x) \text{ which satisfy the Ginzburg-Landau equations } (GL_a): \begin{cases} \frac{1}{\kappa^2} f'' = f(f^2 + q^2 - 1) & \text{in } (-a, a), \\ f'(\pm a) = 0, \\ q'' = qf^2 & \text{in } (-a, a), \\ q'(\pm a) = h_0. \end{cases}$$

In this talk, I will present a complete numerical description of the solutions of (GL_a) in terms of the parameters a , κ and h_0 that we have obtained using the software Auto. We have determined the number, symmetry and stability of solutions for all values of the parameters. In particular, our experiments reveal the existence of two key-points in parameter space which play a central role in the formation of the complicated patterns by means of bifurcation phenomena. This description also allows us to separate the various physically important regimes (type I, type II, nucleation of vortices), to classify previous results in each regime according to the values of the parameters and to derive new open problems.

ALMOG, Yaniv (Technion-I.I.T, Israel)

On the bifurcation and stability of periodic solutions of the Ginzburg-Landau equations in the plane

The linear bifurcation and stability of periodic solutions to the Ginzburg-Landau Equations in the plane are investigated. In particular, we find new infinite families of solutions, which include the few solutions reported in the literature. Then, the vortex structures of these new solutions are examined. In addition, the energies of all possible solutions are approximated in the limit case for which the fundamental cell is a very thin and long rectangle. In that limit, we find that the energy of the solution representing the well-known triangular lattice is the lowest. Finally, we examine the stability of one infinite family of solutions, which include both the triangular and square lattices, in an infinite-dimensional space of perturbations (in contrast to a previous work in which stability is examined only in a finite-dimensional space). We find that in addition to the triangular lattice other solutions are stable as well.

BAUMAN, Patricia (Dept. of Mathematics, Purdue University, W. Lafayette, USA)

A three-dimensional superconductor in a strong magnetic field

We investigate the behavior of a three-dimensional superconducting solid of revolution in a uniform magnetic field. We show that the material exhibits vortex filaments of normal (nonsuperconducting) sites when it is a type II superconductor and the magnetic field is sufficiently large but below an upper critical value. We also describe the nature of the induced magnetic field which is quite different from the two-dimensional case.

CHEN, Zhiming (Institute of Mathematics, Academia Sinica, Beijing, China)

Adaptive Galerkin methods for a dynamical GL model in superconductivity

The time-dependent Ginzburg-Landau model which describes the phase transitions taking place in superconductors is a coupled system of nonlinear parabolic equations. It is discretized semi-implicitly in time and in space via continuous piecewise linear finite elements. A posteriori error estimates are derived for the $L^\infty L^2$ norm by studying a dual problem of the linearization of the original system, other than the dual of error equations. Numerical simulations are included which illustrate the reliability of the estimators and the flexibility of the proposed adaptive method.

DU, Qiang (Hong Kong University of Science and Technology, Hong Kong, China)

Ginzburg-Landau vortices in d -wave superconductors

We discuss some recent Ginzburg-Landau type models for d -wave superconductors. Comparisons between the vortices in the conventional G-L models and that in the d -wave models will be given. Both theoretical and computational studies will be presented.

PAN, Xingbin (Zhejiang University, Hangzhou, China)

Surface nucleation of superconductivity

In this talk we discuss the nucleation phenomenon for a superconductor occupying an arbitrary bounded smooth domain in R^3 . We give an estimate for the value of upper critical field $H_{C_3}(\kappa)$. This estimate, which improves the formula obtained by St. James and De Gennes, shows that curvature of boundary plays an important role in the surface nucleation phenomenon. We also discuss the location of nucleation and estimate the strength of nucleation in terms of the concentration behavior of order parameters. This is a joint work with Kening Lu.

PHILLIPS, Daniel (Purdue University, USA)

Flux creep in High-Tc superconducting materials

We consider the equations modeling flux creep in a high-Tc superconducting wire or tape subjected to periodic applied magnetic field and transport current. We analyze the current distribution through the cross section of the wire and its large time behavior.

This work is joint with P Bauman and M Friesen.

RICHARDSON, Giles W (Ecole Normale Supérieure, France)

The bifurcation structure of a thin superconducting loop with small variations in its thickness

We study bifurcations between the normal and superconducting states, and between superconducting states with different winding numbers, in a thin loop of superconducting wire, of uniform thickness, to which a magnetic field is applied. We then consider the response of a loop with small thickness variations. We find that close to the transition between normal and superconducting states lies a region where the leading order problem has repeated eigenvalues. This leads to a rich structure of possible behaviours. A weakly nonlinear stability analysis is conducted to determine which of these behaviours occur in practice.

STYLES, Vanessa (Oxford Brookes University, UK)

Analysis of mean field models of superconducting vortices in one and two-dimensions

The mean field model of superconducting vortices comprises of a coupling between a hyperbolic and an elliptic partial differential equation involving two variables w and H which respectively denote the vortex density, commonly known as the 'vorticity', and the average magnetic field of the superconducting sample. We study simplified one and two-dimensional forms of this model, and prove the existence of a weak solution and a steady state solution, which takes the form of a free boundary problem. For the one-dimensional model we prove that the weak solution is unique and that it satisfies an entropy inequality. We derive a finite-volume discretization of the one and two-dimensional models. For the one-dimensional model we prove that in the limit as the mesh size and the time step tend to zero, our numerical approximation converges to the unique weak solution of the model. Lastly we introduce some generalisations of the model which deal with nucleation of vorticity at the boundary and flux pinning.

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DOUGLAS, Craig C (University of Kentucky, USA)

Cache based multigrid methods for problems on unstructured grids

All RISC based computers attain high performance using memory hierarchies to make up for memory chips not keeping pace with the speedup of processors. Multigrid combines several standard sparse matrix techniques. We investigate when it makes sense to combine several of the multigrid components into one, using bitwise equivalent, block oriented algorithms. We determine how large (or small) the blocks must be in order for the data in the block to just fit into the processor's primary cache. By re-using the data in cache several times, the savings in runtime can be predicted. Structured and unstructured grids cases are treated.

HENSON, Van Emden (Lawrence Livermore National Laboratory, USA)

Advances in parallelizing algebraic multigrid

The need to solve linear systems on extremely large, unstructured grids has generated interest in creating a scalable parallel algebraic multigrid (AMG) algorithm. Much of AMG can be parallelized in a straightforward fashion, using existing technology. However, the "classical" AMG algorithm selects coarse-grid points in a manner that is inherently sequential. We describe a parallel AMG code, where coarse-grid selection is based on finding independent sets modified by applying certain heuristics. We seek to attain scalability of the convergence factor, so that it remains essentially constant at some reasonable value as problem size and the number of processors increase.

RUGE, John (Front Range Scientific Computations, Inc., USA)

Algebraic multigrid methods for the solution of PDE's: Old and new ideas

Algebraic multigrid methods are designed to solve linear systems arising from discretized PDE's, in the most general case without knowledge of the underlying continuous problem or geometry. This talk will begin by summarizing the "classical" AMG algorithm, developed by Ruge and Stueben. There has been a recent resurgence of interest in AMG due to the need for efficient solution methods for very large problems defined on unstructured meshes. The advantages and shortcomings of the classical algorithm will be discussed, and new ideas for coarsening and interpolation definition, particularly for finite element discretizations, will be presented.

SAUTER, Stefan (Universitaet Leipzig, Germany)

Composite finite elements for problems with jumping coefficients

Composite finite elements allow coarse scale discretizations of PDEs on complicated domains. For standard model problems (Laplace operator with Neumann/Dirichlet boundary conditions), the approximation property holds independently of the size and number of geometric details contained in the domain. These coarse scale discretizations can be used within a multigrid procedure to solve the system of equations on the finest scale. We will introduce composite finite elements for problems with jumping coefficients. The approximation property is proved in various norms. We will show results of numerical experiments showing the convergence behavior of these finite elements in a multi grid algorithm.

CHAPMAN, John N (Department of Physics and Astronomy, University of Glasgow, UK)

Experimental observations of domain structures in patterned magnetic thin films

Magnetic elements with dimensions in the micron and sub-micron regime can be fabricated by electron beam lithography and studied using transmission electron microscopy. Observations of how the domain structure evolves under the application of a magnetic field can be made in real time leading to much useful information on switching mechanisms. The behaviour of isolated elements and arrays of elements can be compared giving insight into the nature of interactions within densely packed element arrays of interest for magnetic information storage. The experimental results also provide a valuable test bed against which the results of micromagnetic modelling can be compared. Once agreement between experiment and theory is realised, modelling can be used advantageously to optimise element geometry resulting in magnetic properties tailored for specific applications.

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OTTO, Felix (University of California at Santa Barbara, USA)

Domain branching in type-I superconductors

A superconducting specimen of type I is placed in an external magnetic field. The sample is a plate oriented perpendicular to field. It is observed that the sample splits into an arrangement of superconducting domains, where the applied field is expelled, and normal domains. We derive the predictions of the Ginzburg-Landau domain theory w. r. t. the average size of these domains, as it scales in the parameters, in particular the strength of the applied field. Our method is a rigorous renormalization of the variational problem. This is joint work with Rustum Choksi and Bob Kohn.

PROHL, Andreas (Christian-Albrechts-Universitaet Kiel)

Analysis of finite element approximation of microstructure in micromagnetics

The magnetization of uniaxial ferromagnetic bodies is described by the solution of a non-convex variational problem, exhibiting microstructure. As it is known from a work of Luskin and Ma, striking upper bounds for the lowest energy for piecewise constant magnetizations can be verified in case the mesh is aligned with the laminated microstructure, but corresponding arguments do not apply to general meshes. In this talk, their results are generalized to general meshes. This goal is reached by considering refined, multiscale branching structures close to the boundary of the domain.

In a second part, the numerical modelling of cubic ferromagnets will be addressed. As a consequence of improved symmetry properties of the ferromagnetic material, improved rates of convergence can be verified for the lowest energy that is obtained in the finite element model.

These results can even be improved on adapted meshes that are refined close to the boundary of the domain and that will be discussed in the talk.

REITICH, Fernando (School of Mathematics, University of Minnesota, USA)

Calculation of the overall magnetic properties of magnetorheological fluids

Magnetorheological fluids (MRF), composed of micron-sized polarizable particles dispersed in a carrier liquid, constitute examples of controllable ("smart") fluids whose rheological properties vary in response to an applied magnetic field. Understanding the magnetic behavior of MRF is crucial to the development of MRF-based devices and it also provides valuable insight into the character of the microstructure responsible for their field-dependent rheology. In this talk we will present results on the calculation of the overall magnetic response of MRF. We will show that effective medium approximations and particle dynamics simulations deliver numerical results that are in good agreement with experimental data and which can, therefore, be used to assist in the design of improved MRF.

SMYSHLYAEV, Valery (Department of Mathematical Sciences, University of Bath, UK)

Variational bounds for assemblages of fine ferromagnetic particles

Variational bounds for the effective magnetic properties of systems of fine interacting magnetic particles are discussed. For a statistically uniform assemblage characterized by the one and two point correlation functions, rigorous bounds on the stored energy are derived by developing a Hashin-Shtrikman type variational approach in the statistical context. This provides variational estimates for the overall magnetization of the system in terms of the statistical properties of the underlying microstructure. This is joint work with A DeSimone, Keipzig.

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ERN, Alexandre (CERMICS, ENPC, France)

Detailed modelling of chemical vapor deposition

Chemical Vapor Deposition (CVD) is an industrially important technique for growing thin layers to be used in optoelectronic devices and semiconductors. CVD involves flowing chemical precursors into a reactor containing a heated substrate where growth occurs. Modelling of the process must account for mixed convective, multidimensional flow inside the reactor, heat transfer phenomena, chemical reactions in the vapor and at the growing surface, and multicomponent transport of gas-phase precursors. In this talk, we discuss recent advances in modelling CVD of a gallium arsenide layer using organometallic and hydride precursors. We present numerical results on layer uniformity and impurity incorporation as a function of operating parameters.

GIOVANGIGLI, Vincent (CMAP/CNRS Ecole Polytechnique, France)

Plane laminar flames with detailed transport and complex chemistry

We consider the governing equations for plane laminar flames as derived from the kinetic theory of polyatomic reactive gas mixtures. An arbitrary number of reversible chemical reactions and the most general form for multicomponent transport fluxes given by the kinetic theory are taken into account. An existence theorem is obtained by first considering a bounded domain and then letting the size of the domain to go to infinity. We establish in particular that the natural entropy production norm associated with multicomponent diffusion is a solution-weighted norm involving mass fractions at the denominator of the mass fraction gradients squared.

MASSOT, Marc (CNRS, Equipe d'Analyse Numérique, Université Lyon 1, France)

Asymptotic stability of equilibrium states for multicomponent reactive flows with detailed transport and complex chemistry

We consider the equations governing multicomponent reactive flows derived from the kinetic theory of dilute polyatomic reactive gas mixtures. Using an entropy function, we derive a symmetric conservative form of the system. In the framework of Kawashima's and Shizuta's theory, we recast the resulting system into a normal form, that is, in the form of a symmetric hyperbolic-parabolic composite system. We also characterize all normal forms for symmetric systems of conservation laws such that the nullspace associated with dissipation matrices is invariant. We then investigate an abstract second order quasilinear system with a source term, around a constant equilibrium state. Assuming the existence of a generalized entropy function, the invariance of the nullspace naturally associated with dissipation matrices, stability conditions for the source term, and a dissipative structure for the linearized equations, we establish global existence and asymptotic stability around the constant equilibrium state in all space dimensions and we obtain decay estimates. These results are then applied to multicomponent reactive flows using a normal form and the properties of Maxwellian chemical source terms.

VOLPERT, Vitaly (University Lyon 1, France)

Influence of natural convection on stability of reaction fronts

Propagation of reaction fronts such as gaseous flames or frontal polymerization can be strongly influenced by convection. We study critical conditions of convective instability for various models and compare theoretical and experimental results. We describe a new type of instability which appears because of interaction of chemical fronts and hydrodynamics and study the influence of convection on the thermal instability.

BUDAEV, Bair V (University of California at Berkely, USA)

What is wrong with the Maliuzhinets function?

The Maliuzhintez' function was introduced in pioneering papers of G D Maliuzhinetz dealing with the problem of diffraction of acoustic waves by wedges with impedance boundary conditions. These problems were reduced to functional difference equations and the required solutions were expressed in terms of products of the meromorphic Maliuzhinetz function, which added elegance to the obtained analytically closed-form solutions. Unfortunately, elementary analysis shows that analytical properties of the Maliuzhinetz functions are less attractive than the behaviour of the final solution of functional equations, and that computations based on this theoretically perfect function may be compared with the computation of $\sin(x)$ by multiplying two Gamma functions of arguments x and $1 - x$. In the talk an improved version of the "Maliuzhinetz" function will be suggested.

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LAWRIE, Jane B (Brunel University, UK)

On the diffraction of waves in wedges with contrasting material properties

The study of wave reflection and diffraction in wedges has a long and interesting history, with particular interest paid to various canonical problems. One such model is that of adjoining homogeneous wedge regions of differing material properties such as, for fluid mechanical applications, density and sound speed variations; this dielectric wedge problem also has important applications in electromagnetic wave theory. Mathematical approaches have centred on a variety of methods, such as application of the Kontorovich-Lebedev transform and the Sommerfeld integral representation. This talk will show that the latter approach can be used successfully on the dielectric wedge model, and gives explicit details of the diffracted field and multiply-reflected wave terms for a particular choice of the material constants. This is a joint work with I D Abrahams, University of Manchester, UK, and A M J Davis, University of Alabama, USA.

LYALINOV, Michael A (Dept. Mathem. Physics, St Petersburg University, Russia)

Coupled Maliuzhinets' equations and their direct reduction to Fredholm type integral equations

In modern electromagnetic diffraction theory by wedges the boundary-value problems with different vectorial boundary conditions are usually reduced to systems of coupled Maliuzhinets' functional equations. We consider an approach which is based on the direct reduction of the problems to the second kind integral equations. As an important example we consider the problem of electromagnetic diffraction of an obliquely incident plane wave by an impedance wedge. The functional equations are transformed to two independent difference equations of the second order with the variable coefficients. By use of the theory of S-integrals the reduced difference equation is transformed to the second kind integral equation which can be studied in the appropriate functional space.

NORRIS, Andrew N (Rutgers University, USA)

Wiener-Hopf problems associated with thin plate diffraction

Several problems associated with structural wave diffraction on thin plates are described and their solutions developed. The first is scattering of flexural waves from a semi-infinite crack. The classical Kirchhoff theory leads to a scalar Wiener-Hopf problem with a relatively explicit solution: the kernel involves only a finite integral. The same level of difficulty holds for the dual problem of scattering from a semi-infinite rigid strip. The crack problem is then discussed in the context of Mindlin plate theory, for which a matrix Wiener-Hopf system is obtained. Strategies for its solution are discussed. Finally, diffraction from corners of wedge-shaped plates will be discussed.

OSIPOV, Andrey V (St Petersburg State University, Russia)

New algorithms for the computation of Malyuzhinets' special function

The paper presents new numerical algorithms for the computation of a special function introduced by G D Malyuzhinets in the 50th as a meromorphic solution to a system of difference equations occurring in the theory of diffraction of waves by an imperfectly reflecting wedge. The proposed algorithms employ and combine various analytical representations of the Malyuzhinets function, including its finite product and integral representations, as well as its large argument expansion. In total, five numerical algorithms have been developed and implemented as FORTRAN subroutines differing from each other in accuracy and computational speed. This is a joint work with V Stein.

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LOGINOV, Boris V (Ulyanovsk State University, Russia)

Determination of bending eigenforms and asymptotics of bifurcating solutions at the divergence of rectangular plate

The problem about the deflection of rectangular plate flowed around by supersonic gas flow (see Vol'mir A.S., *Stability of deformable systems*, M., Nauka, 1967-984p. and Loginov B.V., *Plate divergence as bifurcational problem with symmetry*, Algebraic and analytic methods in differential equations-Proceedings Internat. Conference. Oryol, 14-19.11.1996, p.90-93) is considered. This problem is describing by von Karman's system of nonlinear equations and is bifurcational with Mach number M as bifurcational parameter. The main difficulties consist of the branching points determination and corresponding zero-subspace of linearized operator. The cases of hinged fastening of the plate along Oy axis and various fastenings along Ox axis are considered. Here the Fourier separation variables method leads to two-point boundary value problems for ordinary differential equation of the fourth order. It is proved that the corresponding characteristic equation has two negative $-\alpha, -\beta$ and a pair of complex-conjugate roots $\gamma \pm i\delta$ ($\alpha + \beta = 2\gamma, \delta > 0$). The critical values of the Mach number $\sigma = \sigma(M^*)$ and bifurcating solutions asymptotics by small deviation $M - M^*$ are expressing through the functions of parameter γ .

SIDOROV, Nikolay A (Irkutsk State University, Russia)

On asymptotic bifurcation directions for Vlasov-Maxwell system in the plasma theory

For the Vlasov-Maxwell system sufficient conditions are obtained for the existence of asymptotic direction of multiparametric bifurcation, corresponding to the distribution function of the special form. It is assumed that the values of the scalar and vector potentials of electromagnetic fields are prescribed at the domain D. The stationary system is reduced to the quasilinear elliptic equations. The asymptotic bifurcation direction is analyzed. The bifurcation Lypunov-Schmidt system is derived and studied for the solutions. The asymptotics of branching solutions of the Vlasov-Maxwell system are constructed in a neighborhood of the bifurcation points in the case of a circular cylinder.

TRENOGIN, Vladilen A (Department of Mathematics, Moscow State Steel and Alloys Institute, Russia)

Bifurcation equation for one-parametric families of solutions of nonlinear equations

Let operator $F(x)$ maps the neighborhood of the point x_0 from X into a neighborhood of space Y zero and $F(x_0) = 0$. We consider the situations when the initial equation $F(x) = 0$ has near the point x_0 several one-parametric families solutions (see Trenogin V.A., *Funct. Anal. and Appl.*, v.(1), 1998 and *Vestnik RUDN, ser. Math.*, v.3(1), 1996). Suppose $F(x)$ differentiable, $B = -F'(x_0)$, $N = N(B)$. We do not suppose finite dimensionality of N . We obtain branching equation (BE) (see Trenogin V.A., *Vestnik RUDN, ser. Math.*, v.3(1), 1996 and *Functional Analysis*. Nauka, Moscow, 1980). Next we obtain the variant of BE for all branches of solutions tangent to the vector from N . Asymptotic representation and iterational schemes are investigated. If the initial equation is presented with numerical parameter then from our results some results of (see Sidorov N.A., *Math. Sbornik.*, v.186 (2), 1995) are followed.

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BORCEA, Liliana (Rice University, USA)

Matching pursuit for imaging high contrast conductive media

We consider the highly nonlinear inverse problem of imaging a high contrast electrical conductivity, given the currents and voltages (the Neumann to Dirichlet map) at the boundary. For large contrast media, we show that the current flow can be approximated by current in an asymptotic resistor network. Furthermore, we show that the Neumann to Dirichlet map of a high contrast continuum is asymptotically equivalent to the Neumann to Dirichlet map of the resistor network. We discuss the construction of the asymptotic resistor network for arbitrary boundary excitations and high contrast media. Based on the asymptotic theory, we use a matching pursuit approach to solving the high contrast inverse problem, where the library of functions is constructed in accordance with the previously developed asymptotic theory. We present various numerical results and show comparisons with matching pursuit with other libraries of functions such as Gaussians and wavelets.

DRUSKIN, Vladimir (Schlumberger-Doll Research, USA)

Gaussian spectral rules for three-point second differences and their application to numerical solution of PDEs

A special sequence of grid steps is found which yields exponential superconvergence of the Neumann-to-Dirichlet map using standard second order finite-difference schemes. Our technique is based on a known connection between Padé approximations, the Stieltjes moment problem, the Lanczos method and the inverse spectral (impedance) problem. We apply this approach to solve some two-dimensional elliptic and wave boundary value problems. Our numerical experiments exhibit exponential and even superexponential convergence at prescribed points, where the cost per grid node is close to that of the standard second order finite-difference scheme. For the wave problems, including the two-dimensional wave equation with piecewise-constant coefficients, our mesh demonstrates high accuracy with slightly more than two grid points per wavelength, compared to more than twenty points per wavelength for the standard five-point scheme. This is a joint work with Leonid Knizhnerman and Sergey Asvadurov.

INGERMAN, David (Courant Institute of Mathematical Sciences, USA)

Characterizations and approximations of planar Dirichlet-to-Neumann maps

A positive function (conductivity) on a planar domain induces the *Dirichlet-to-Neumann* or *Steklov* map from potentials on the boundary of the domain to boundary currents. We will talk about characterizations of the Dirichlet-to-Neumann maps with an emphasis on the case of radially symmetric conductivities. In this case we completely characterize the set of the discrete and continuous Dirichlet-to-Neumann maps in terms of their kernels and spectra. The characterizations and our solution of the discrete inverse problem lead to new ways of Dirichlet-to-Neumann map discrete approximations that do not require the knowledge of the conductivity.

ISAACSON, David (Math Dept. RPI, Troy, USA)

Problems in electrical impedance imaging

Electrical impedance imaging systems apply electric currents to the outside of a body and measure the voltages that result. From this data they reconstruct and display approximations to the electrical conductivity and permittivity inside the body. Images from the ACT3 system designed to monitor patients for ventilation and perfusion as well as screen for breast cancer will be shown. The Spectral properties of the Dirichlet to Neuman Operator that motivated the design of the mesh used for reconstructing these images will be presented.

KNIZHNERMAN, Leonid (Central Geophysical Expedition, Russia)

Optimal network approximation for large spectral intervals

Druskin and Knizhnerman found a special sequence of grid steps which yields exponential superconvergence of the Neumann-to-Dirichlet map using the standard second order finite-difference scheme based on a three-point approximation of the second derivatives. We show, that the exponential convergence rate of that grid is still not optimal and present an algorithm and asymptotical error estimates for the optimal grid. For a large spectral interval the optimal exponential convergence rate is proportional to the inverse of the logarithm of the condition number of the interval. We use known error bounds for rational approximations obtained by methods of potential theory.

MORROW, Jim (University of Washington, Seattle, USA)

Continuous and discrete Dirichlet-to-Neumann maps for a plane region

The Dirichlet-to-Neumann map for the electrical conductivity equation on a simply connected plane region has an alternating property, which may be considered as a generalized maximum principle. This property can be used to construct a discrete approximation to the continuous problem. The discrete problem can then be solved to give an approximation to the original problem.

MOSKOW, Shari (University of Florida, USA)

Three point finite difference schemes and the spectral Galerkin method

Druskin and Knizhnerman have developed a three point difference discretization of a second order ODE which yields exponential convergence of the Neumann to Dirichlet map. Here we show that this discrete Neumann to Dirichlet map obtained by Pade approximation is actually the same as one would obtain from a Galerkin method, but in contrast with Galerkin the resulting linear system is sparse. We also discuss how this method may be applied to equations with variable coefficients.



ASANO, Tetsuo (JAIST, Japan)

An efficient and robust algorithm for enumerating digital line components

Hough transform is a popular method for detecting digital line components in a binary image. The popularity comes from the simplicity of the notion of voting into parameter plane. In this talk we discuss about the computational complexities of the line detection problem under the constraint that every line must be detected and propose an efficient and robust algorithm by effective use of geometric computation.

FORTUNE, Steven J (Bell Labs, Lucent Technologies)

The reliable implementation of geometric algorithms using exact arithmetic

Implementing geometric primitives with exact arithmetic is attractive, since it avoids the numerical difficulties that result from floating-point arithmetic. Exact arithmetic is feasible for many algorithms involving linear objects in dimensions two and three, since the required arithmetic bit-length is relatively modest. An implementor must consider many issues, including representation of numeric values, choice of geometric primitives, recasting of algorithms to constrain arithmetic bit-length, and the clean up of actual, possibly noisy input data to an consistent surrogate input data. This talk will survey the emerging methodology of exact-arithmetic implementation, describe experience with actual implementations, and indicate open problems.

IMAI, Hiroshi (Department of Information Science, University of Tokyo, Japan)

Degeneracy issues in integer programming approach to optimum triangulations of points in two and three-dimensional space

Two- and three-dimensional triangulations are used as fundamental structures in mesh generation for finite element mesh and voxel computation for computer graphics. In this talk, we first mention an integer-programming approach to this problem with some geometric characterization. Then, we discuss computational issues related to degeneracies in many respects. Through this approach, we establish an efficient way of handling this fundamental geometric structure from the viewpoint of optimization and computational geometry.

IMAI, Toshiyuki (Wakayama University, Japan)

Symbolic perturbation based on Gröbner basis

A method to treat the degeneracies for geometric algorithms is proposed. This is a kind of symbolic perturbation method like other conventional ones. When it is implemented, additional codes are relatively small by this method. This method is applicable as long as the determinants for the structures of figures are polynomials even if these polynomials are given implicitly. This method is also easy to be applied the programs which are already implemented. These are because this method mainly replace the data structures of the program while conventional ones modify the program itself. This method is based on the Gröbner basis with certain properties. The arbitrariness of this method is also proved.

NAEHER, Stefan (Martin-Luther Universitaet Halle, Germany)

Computational geometry with LEDA and CGAL

The availability of a library providing implementations of recent and advanced techniques can make a tremendous difference for the technology transfer from theory to practice. The talk gives an overview on two related projects that aim to make computational geometry available for (industrial) application. LEDA (Library of Efficient Data types and Algorithms) provides a platform for combinatorial and geometric computing. It is known for its strong combinatorial part and due to much progress concerning geometric computation in the last three years it now has a solid geometric part as well. LEDA is commercial, but still free for academic use (see <http://www.mpi-sb.mpg.de/leda> for exact terms). CGAL (Computational Geometry Algorithms Library) is a recent European research project concentrating on geometry. Since CGAL is designed to be modular and flexible with respect to lower implementation layers, it is easy to make use of the LEDA's exact arithmetic in CGAL and to combine CGAL with the solid geometry kernels of LEDA.

OHSAWA, Akira (Chubu University, Japan)

2D space model for general robust geometric algorithms

Robustness is achieved by keeping topological consistency. The 2D topology is represented with a directed planer graph represented by pointer-pairs. The separated representation between the topology and the geometry allows maintaining topological consistency regardless of calculation errors and degeneracy. "Topological staggering" technique eliminates the degeneracy problems. A variety of geometrical algorithms run fast: updating, closed area detection, set operations, hidden-line/surface removal, collision detection, and so on. The 2D program was successfully implemented and running in a PCB CAD system. This method could be expandable to 3D geometry.

SUGIHARA, Kokichi (University of Tokyo, Japan)

Scientific computation using topology-oriented geometric data

Topology-oriented methods for robust geometric computation can guarantee their outputs to be topologically consistent, but they may contain geometrical disturbance. However, even though they include geometric disturbance, they can be used in practical applications without any serious problems if the application methods are also revised in a topology-oriented manner. The examples of such applications include interpolation based on the Voronoi diagram and finite element methods for partial differential equations.

GRAHAM, Ivan G (University of Bath, UK)

Implementation of fast integration methods in 3D boundary elements

In this talk we describe the implementation of the fast integration techniques which were discussed in the talk by W. Hackbusch. In these techniques most of the stiffness matrix arising in a boundary element method is computed by node-based quadrature rules, the weights of which have to be computed in a first phase of the matrix assembly process. This constitutes an $O(N)$ process, which in practice is a small fraction of the overall assembly time. Once these weights are computed the matrix is assembled by an adaptive routine which uses the node-based quadrature rules wherever possible and only conventional element-based rules for a small number of singular or nearly singular elements. We describe the general principles behind the implementation of this algorithm and illustrate these with computational experiments involving boundary integral equations on a selection of smooth and non-smooth surfaces. The experiments show that the theoretical results given in W. Hackbusch's talk are realisable in practice for a variety of problems, even including the strongly anisotropically refined meshes commonly used for approximation of edge singularities.

The talks of Hackbusch and Graham in this minisymposium describe results jointly obtained by I.G. Graham, W. Hackbusch and S.A. Sauter.

HACKBUSCH, Wolfgang (Praktische Mathematik, University of Kiel, Germany)

Fast integration in 3D boundary element methods

In the practical implementation of the boundary element method in 3D the formation of the stiffness matrix (containing surface integrals involving the kernel function of the integral operator) often forms a dominant part of the computation time. For N degrees of freedom the cost of assembling the complete matrix is CN^2 with C moderately large and depending on the number of kernel evaluations used by the integration routine. In this work we describe a new fast quadrature method for approximating the stiffness matrix which reduces this cost. For example, in the case of continuous piecewise linear basis functions on a mesh with N nodes, the new method computes the stiffness matrix using $N^2 + O(N)$ kernel evaluations. The N^2 term comes from the fact that most of the matrix is computed using novel rules which just use kernel evaluations at pairs of nodes, with the lower order term coming from conventional rules applied to the small remaining part of the matrix. The computed (approximate) stiffness matrix is guaranteed to be sufficiently accurate so as to preserve the known theoretical convergence properties of the numerical method. In this talk we will describe the essential ideas behind this method and we will review recent theoretical results concerning its stability, convergence and complexity.

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HAYAMI, Ken (Department of Mathematical Engineering, Graduate School of Engineering, University of Tokyo, Japan)

Multipole method for 3-D elastostatics

We use multipole expansions of fundamental displacement and traction around the centre of a cluster of elements in the far-field. This reduces memory and work for matrix-vector multiplications in iterative solvers for BEM. Fundamental displacement is expressed as linear combinations of $1/r$ and spatial derivatives of r , the distance between observation and field points. Multipole expansions of the latter are derived from the known expansion for the former in terms of spherical harmonics. This further reduces computational costs compared to polynomial-type expansions, since the expansions are essentially two-dimensional instead of three. An efficient implementation and its complexity will be discussed. This is a joint work with Professor Stefan A Sauter, Universität Leipzig.

SAUTER, Stefan (University of Leipzig, Germany)

Fully discrete panel clustering

Boundary element discretizations of integral equations typically lead to a system of linear equations with a dense coefficient matrix. Since the dimension N of this matrix can be very large iterative solvers should be applied for its solution. For the realization of iterative solvers, it is sufficient to perform matrix vector multiplications; the coefficients of the matrix are not explicitly needed. The panel clustering method approximates a matrix vector multiplication with $O(N(\log N)^k)$ operations (instead of N^2). However, the implementation of the panel clustering algorithm is not trivial and various parts of the algorithm are based on analytic formulae and recursive algorithms which have to be modified for different applications (e.g. different integral kernels). In our talk, we will present a fully discrete version of the panel clustering algorithm and discuss the complexity of the method.

SCHWAB, Christoph (ETH Zurich, Switzerland)

Wavelet Galerkin algorithms for boundary integral equations

The implementation of a fast, wavelet-based Galerkin discretization of second kind integral equations on piecewise smooth surfaces $\Gamma \subset \mathbb{R}^3$ is described. It allows meshes consisting of triangles as well as quadrilaterals. The algorithm generates a sparse, approximate stiffness matrix with $\mathcal{N} = O(N \log^2 N)$ nonvanishing entries in $O(N \log^4 N)$ operations where N is the number of degrees of freedom on the boundary while essentially retaining the asymptotic convergence rate of the full Galerkin scheme. A new proof of the matrix-compression estimates is given based on derivative-free kernel estimates. The condition number of the sparse stiffness matrices is bounded independently of the meshwidth. The data structure containing the compressed stiffness matrix is described in detail: it requires $O(\mathcal{N})$ memory and can be set up in $O(\mathcal{N})$ operations. Numerical experiments show that the asymptotic performance estimates apply for moderate N . Problems with $N = 10^5$ degrees of freedom were computed in core on a workstation. The impact of various parameters in the compression scheme on the performance and the accuracy of the algorithm is studied.

CHELMINSKI, Krzysztof (Darmstadt University of Technology, Germany)

On initial-boundary value problems in the theory of inelastic deformation of metals

Systems of equations describing inelastic deformation of metals consist of partial differential equations resulting from mechanical balance laws and of a set of so called constitutive equations, which are always dependent of the material under consideration. One way to derive the constitutive relations is to assume that there exists a finite set of internal variables, whose evolution uniquely determine the state of the material. Therefore in the literature we find constitutive equations in the form of ordinary (often nonlinear) differential equations or differential inclusions for the internal variables. Thus we study here a linear system of partial differential equations coupled with a nonlinear system of ordinary differential equations (or general differential inclusions). H.-D. Alber defined the class of constitutive relations "of monotone type", for which the natural mathematical tool to study such equations is the theory of evolution equations for monotone operators. He proved existence and uniqueness of strong, global in time solutions for all constitutive equations of monotone type provided the coercivity assumption for the free energy function. However there are many examples of constitutive equations for which the above assumption fails. We prove existence and uniqueness of strong global in time solutions without the coercivity assumption for the free energy function. We approximate noncoercive models by a sequence of coercive problems and prove the convergence result.

RASCLE, Michel (Université de Nice, France)

Global L^2 solutions to dynamical elasto-plasticity

The talk concerns essentially - but not uniquely - the 1D elasto-plastic problem (EP), with so-called *isotropic* hardening, seen as the zero-relaxation limit $\epsilon \rightarrow 0$ of

$$\partial_t v - \partial_x \sigma = 0,$$

$$\partial_t \sigma - \partial_x v = -(\epsilon)^{-1} \operatorname{sgn}(\sigma) (|\sigma| + g(\gamma) - 1)_+,$$

$$\partial_t \gamma = -(\epsilon)^{-1} (|\sigma| + g(\gamma) - 1)_+.$$

Here, v is the velocity, $\sigma := \epsilon_e$ the stress, with ϵ_e and ϵ_p the elastic and plastic strains, $-\gamma$ is the accumulated plastic strain, and function g , increasing and convex, describes the plastic yield curves, which are assumed to be concave in traction and convex in compression. The striking fact is that this last property, and the irreversibility of plastic evolutions, preclude the existence of plastic *shocks*. I will first recall how this property allows to prove the existence and uniqueness of global solutions to (EP), even in 3D, in Sobolev spaces like H^1 [Nouri-Rasclé, SIAM Math Anal, 1995]. I will then show how one can define (weak) L^2 solutions to (EP), although this problem is an evolution variational inequality of the form $\langle \partial_t U + \partial_x AU, V - U \rangle \geq 0$, which *a priori* has no meaning for L^2 solutions. Again, the crucial point is that the only discontinuities must take place in the elastic regime. In particular, the theory allows to nicely recover the unique solution of the Riemann Problem.

SEDLAN, Konstantin (Universitaet Gesamthochschule Kassel, Germany)

Nonlinear viscoelasticity of elastomers: Constitutive modelling and experimental identification

One- and two-dimensional tension-torsion experiments on circular cylinders made of filled rubber are presented. The experiments motivate the proposal of a constitutive model of nonlinear finite viscoelasticity. The equilibrium stress is described by means of an isotropic strain energy function. The overstress decomposes into a series of generalized Maxwell elements. The viscosities in these elements depend on further internal variables in order to allow for thixotropic effects as suggested by the experimental data. Numerical simulations, based on a set of identified material parameters, demonstrate the ability of the constitutive model to represent the observed phenomena.

SOFONEA, Mircea (Université de Perpignan, France)

Variational analysis of some contact problems for elastic-visco-plastic materials

We consider a number of quasistatic problems which describe the frictional contact between an elastic-visco-plastic body and a foundation. The contact conditions are nonstandard and may include normal compliance, damped normal response and wear. The material's constitutive law may involve internal state variables, which in particular, may describe the evolution of the system's damage. We obtain weak formulations for the models and prove existence and uniqueness results. The proofs are based on the theory of evolution variational inequalities and fixed point arguments. We also consider numerical approximations of the problems and derive error estimates for both spatially semidiscrete and fully discrete schemes.

BOSSAVIT, Alain (Électricité de France, France)

What do we mean by "The symmetries of an equation"?

Symmetry means equivariance with respect to some group action. But one can see, from familiar examples with structures, that at least two kinds of group actions are to be considered: not only those which describe the geometrical symmetry of the structure, but those inherent to symmetries in the elasticity equations themselves, which are more elusive. Some formal elaboration of the concept of symmetry is needed to sort this out, and it should bring rewards (as it did in the field of electromagnetism, with which some analogies can be made). We propose a seemingly suitable framework, and use it to, so to speak, "peel out" the symmetry group of a given problem. One may thus distinguish how the (very different) symmetries of the underlying space, of the material properties, of the structure's shape, and of things such as (when relevant) the finite element mesh, contribute to the symmetry group of the final (computer implementable) problem. Some applications to situations where symmetry is partially lost (mode localization, etc.) are suggested.

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CONNELLY, Robert (Cornell University, USA)

Cataloging stable symmetric tensegrity structures

A tensegrity structure is a collection of struts in compression held rigidly in place by a collection of cables in tension. A basic question is to tell whether this structure remains stable as the stress is increased relative to its stiffness. One way to do this is to calculate a certain n -by- n symmetric matrix Ω , the stress matrix, where the number of points is n . If Ω is positive semi-definite of maximal rank, then the tensegrity structure is stable. If further the tensegrity structure is so symmetric that the group of rigid congruences of the structure is transitive on the vertices, then Ω decomposes into much smaller symmetric matrices corresponding to the irreducible representations of the group of symmetries. In fact it is possible to catalogue all the configurations of such highly symmetric tensegrities for all the point groups of three-space for all the combinatorial choices of connecting the cables, when there are say only two transitivity classes of cables and one class of struts. Some models and pictures from the catalogue will be shown.

GUEST, Simon D (Department of Engineering, University of Cambridge, UK)

A symmetry viewpoint of structural mechanics

Symmetry is a common attribute of both natural and engineering structures. Despite this, and in contrast to structures on a molecular scale, the application of symmetry arguments to the structural mechanics of macroscopic structures is still a novelty. This paper will review some recent work in this area, and will show some of the insights into structural mechanics that can be obtained through careful symmetry arguments.

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FUKUDA, Isamu (Dept. of Architecture, Kokushikan University, Japan)

Blow-up of solutions of semilinear parabolic equations with localized reactions

Consider the initial-boundary value problem (P) $u_t = u_{xx} + f(u(0, t))$, $(x, t) \in (-1, 1) \times (0, T)$, with $u(\pm 1, t) = 0$ and $u(x, 0) = u_0(x)$, where $f(s) \in C^2(\mathbb{R})$ and $f(s) \geq 0$. Problem (P) describes some chemical phenomena in which the nonlinear reaction in a dynamical system takes place only at a single point. Regional blow-up theorems have been proved under the suitable conditions by Chadam-Pierce-Yin. In the case $f(s) = s^p$, the growth rate of blow-up solutions near the blow-up time has been obtained by Wang-Chen. In this talk, we will give the growth rate of blow-up solutions for the problem (P) with $f(s) = e^s$.

IDOGAWA, Tomoyuki (Dept. of Electronic & Information Systems, Shibaura Inst. of Tech., Japan)

On the projection to a certain convex set in $H_0^1(\Omega)$

In this talk, we consider a projection mapping P_K from $H_0^1(\Omega)$ into a convex closed subset K which is defined by $K := \{v \in H_0^1(\Omega) \mid \|\nabla v\|_{L^\infty(\Omega)} \leq 1\}$, where Ω is a bounded domain with a smooth boundary. This projection mapping appears in a treatment of elasto-plastic torsion problem by a variational method. We will propose an iteration algorithm to get $P_K u \in K$ for a given $u \in H_0^1(\Omega)$ and show the convergence property of this iteration.

KOJO, Tomomi (Dept. of Machinery & Control Systems, Shibaura Inst. of Tech., Japan)

Weak solutions for some nonlinear differential equations in a Hilbert space

We prove the well-posedness of the initial value problem for some nonlinear differential equations in a Hilbert space H . Equations of the form (E): $(I + B)\frac{du}{dt} + Au = f$ is considered, where A and B are nonlinear and linear operators acting in H respectively. We construct weak solutions of this problem under suitable conditions on A and B . The IVP for the abstract equation (E) describes, as an application, the IBVP for some nonlinear PDEs appearing in several physical problems including the propagation of long waves of small amplitude, soil mechanics, glaciology and so on.

SUZUKI, Ryuichi (Dept. of Mechanical Engineering, Kokushikan University, Japan)

Existence and nonexistence of local or global solutions of quasilinear degenerate parabolic equations

We consider the existence and nonexistence of local or global solutions of the Cauchy problem of $u_t - \Delta u^m = K(x)u^p$, where $p > m \geq 1$, $K(x) \geq 0$, $\in L_{loc}^\infty(\mathbf{R}^N)$. When $m = 1$ and $K(x) = |x|^\sigma$ for $|x| > R > 0$ ($\sigma \in [-\infty, \infty)$), these problems have been studied by many authors. Especially Pinsky showed recently, the interesting results which said that $p_{1,\sigma}^* = 1 + \{2 + \max\{\sigma, -N\}\}/N$ ($\sigma > -2$) is the cutoff number between the blow-up and the global existence cases and $p_{1,\sigma}^*$ belongs to the blow-up case. In this talk, we extend these results completely to the case where $m \geq 1$ and $K(x)$ is a more general function which may vanish in a cone.

TSUTSUMI, Masayoshi (Dept. of Applied Physics, Waseda University, Japan)

Penalty method for variational inequalities and its error estimates

Penalty method in an abstract form for variational inequalities is discussed. Moreover, error estimates of solutions of penalty problem for a variational inequality is obtained.

BERNIS, Francisco (Universidad Autonoma de Madrid, Spain)

Higher order degenerate parabolic equations in lubrication theory

We consider the fourth-order nonlinear degenerate parabolic equation $h_t + (h^n h_{xxx})_x = 0$ and some of its variations. This equation arises in lubrication models for thin viscous films and spreading droplets as well as in the flow of a thin neck of fluid in a Hele-Shaw cell. The purpose of this lecture is to present context information, interrelationships and reflections on some recent results.

FILA, Marek (Comenius University, Slovakia)

Boundedness of global solutions to degenerate parabolic equations

We consider degenerate parabolic equations (of porous medium type) for which blow-up in finite time may occur for "large" initial data while global solutions also exist for "small" initial data. We give sufficient conditions under which every global solution stays uniformly bounded.

GARCKE, Harald (Institut für Angewandte Mathematik, Universität Bonn, Germany)

On fourth order degenerate diffusion equations - theory and numerical simulation

Degenerate parabolic diffusion equations of the form $u_t + \operatorname{div}(u^n \nabla \Delta u) = 0$, $n > 0$ describe the evolution of a thin viscos film driven by surface tension. These equations are derived from a free boundary problem for the Navier-Stokes equations via a lubrication approximation using the facts that the film is thin and viscos. The quantity u describes the height of the film. In my talk I will speak on qualitative features like the property of finite speed of propagation, a regularization property and the long time behaviour of solutions. In particular I shall demonstrate that there are solutions to initial data which are nonnegative Radon measures. Finally, we will introduce a finite element method to approximate solutions numerically. Via numerical simulations we will illustrate some qualitative features like the development of singularities, waiting time behaviour and convergence to selfsimilar profiles.

GRÜN, Günther (Institute for Applied Mathematics, University of Bonn, Germany)

Nonnegativity preserving convergent schemes for thin film equations

We present finite element schemes for fourth order degenerate parabolic equations that arise e.g. in lubrication theory for the time evolution of thin films of viscous fluids. Discretizing the arising nonlinearities in a subtle way enables us to establish discrete counterparts of the essential integral estimates known from the continuous setting. As a consequence, results on nonnegativity of discrete solutions follow in a natural way and the numerical cost in each timestep mainly reduces to the solution of a linear system involving a sparse matrix. Furthermore, by introducing a timestep control that makes use of an explicit formula for the normal velocity of the free boundary, we keep the numerical cost for tracing the free boundary low. Finally, we present convergence results and some characteristic numerical experiments. This is joint work with Martin Rumpf, Bonn.

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HORSTMANN, Dirk (Mathematisches Institut der Universität zu Köln, Germany)
Blowup results for solutions of a parabolic system modelling chemotaxis
 In this lecture we consider the so-called Keller-Segel model

$$\begin{aligned} a_t(x, t) &= \nabla \cdot (\nabla a(x, t) - \chi a(x, t) \nabla c(x, t)), & x \in \Omega \subset \mathbb{R}^2, & t > 0 \\ c_t(x, t) &= k_c \Delta c(x, t) - \gamma c(x, t) + \alpha a(x, t), & x \in \Omega, & t > 0 \\ \partial a / \partial n &= \partial c / \partial n = 0, & x \in \partial \Omega, & t > 0 \\ a(x, 0) &= a_0(x), & x \in \Omega & \\ c(x, 0) &= c_0(x). & x \in \Omega, & \end{aligned}$$

We prove the existence of radially symmetric initial data for which the solution of this model blows up in finite or infinite time. For the proof we assume that Ω is a disk, $\gamma = 0$ and $\alpha \chi \int_{\Omega} a_0(x) dx > 8\pi k_c$, where $(\alpha \chi \int_{\Omega} a_0(x) dx) / k_c$ is not equal to a multiple of 8π . In a second result we show that if the solution blows up in the nonradial case, the blowup must happen at the boundary of Ω .

SOUPLET, Philippe (Département de Mathématiques, Université de Picardie, INSSET, France, and Laboratoire de Mathématiques Appliquées, Université de Versailles, France)

Blow-up and global existence in a reaction-diffusion model with free boundary

We consider a one-phase Stefan problem for the heat equation with a nonlinear reaction term. We first exhibit an energy condition, involving the initial data, under which the solution blows up in finite time in L^∞ norm. We next prove that all global solutions are bounded and decay uniformly to 0, and that either: (i) the free boundary converges to a finite limit and the solution decays at an exponential rate, or (ii) the free boundary grows up to infinity and the decay rate is at most polynomial. Finally, we show that small data solutions behave like (i), and that some global solutions of type (ii) also exist.

ZEIDLER, Martin (RWTH-Aachen, Aachen, Germany)

Localized blow up phenomena

We consider the following degenerate parabolic initial boundary value problem
 $u_t = u^p(\Delta u + u), \quad x \in \Omega, t > 0,$
 $u(x, t) = 0, \quad x \in \partial \Omega, t > 0,$ where $\Omega \subset \mathbb{R}^n$ is a smooth bounded domain and $u_0 \in C^1(\bar{\Omega})$ is
 $u(x, 0) = u_0(x), \quad x \in \Omega,$

positive in Ω . In the general case $p > 1$ blow-up occurs in finite time T if the Dirichlet-problem for $-\Delta$ has the first eigenvalue λ_1 less than 1. We investigate the existence and uniqueness of smooth positive solutions within the time interval $[0, T)$. In the case $p = 2$ Friedman and McLeod proved that the blow-up set S (i.e. $S := \{x \in \Omega \mid \exists (x_k, t_k) \rightarrow (x, T) \text{ such that } u(x_k, t_k) \rightarrow \infty\}$) has positive Lebesgue measure under the additional assumption $\Delta u_0 + u_0 \geq 0$. This proof can be carried over to the general case $p > 1$. Our main interest is to explore where and how blow-up occurs, i.e. to describe the size (and the shape) of S and the asymptotic behaviour of u in a neighbourhood of a blow-up point.

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CHORIN, Alexandre J (University of California, Berkeley, USA)

A new formulation of the near-equilibrium theory of turbulence

A status report will be presented on a numerical approach to turbulence theory. The main idea is to take a distinguished limit of a dense set of impulse loops, in a way that brings out a connection between turbulence and critical phenomena. The approach yields a probability density for turbulence fluctuations that includes intermittency, organized structures, and a Kolmogorov spectrum. This is a joint work with G I Barenblatt.

CORTEZ, Ricardo (Tulane University, USA)

Computation of immersed boundary motions using impulse

The formulation of the Navier-Stokes equations in terms of impulse density is used to derive a Lagrangian numerical method that combines vorticity and impulse. The method is used to simulate the motion of flexible membranes moving in a high Reynolds number flow. Two examples of such applications, the motion of a fluid surrounding an elastic membrane and the motion of a swimming organism, will be presented.

OSELEDETS, Valery (Moscow State University, Russia)

Some remarks on velocity - impulse formulation

The talk is concerned with some problems related to velocity - impulse formulation.

RUSSO, Giovanni (Dipartimento di Matematica, Università dell'Aquila, Italy)

Impulse formulation of the Euler equations and fluid-membrane interaction

The gauge freedom of the Euler equation written in impulse form is explored. Numerical methods to compute the impulse variable in a variety of gauges are presented and results in 2D and 3D are shown. A particular gauge gives a Hamiltonian formulation of incompressible fluid dynamics. This formulation is applied to study the interaction of a fluid with a membrane in two and three dimensions. The analogy with vortex formulation and potential theory is emphasized. Linear analysis is performed in 2D and 3D for axisymmetric flow. Numerical schemes based on this formulation have interesting conservation properties. Numerical results are compared with linear analysis.

SUMMERS, David M (Napier University, UK)

Numerical impulse generation at a solid boundary

Incompressible fluid flow can be represented in terms of an evolution of impetus (or velocity). Treated as a field of compact support, the variable in question is dimensionally an 'impulse density'. In the context of viscous flow, the boundary condition $\mathbf{u} = 0$ at a stationary solid wall can be expressed in terms of decompositions of the impetus variable there; these, in turn, can be interpreted as representing the imparting of impulse to the flow due to boundary forces. The decomposition can be chosen to represent components of impulse tangential to the wall, or alternatively, normal to the wall. Numerical Lagrangian models of flow evolution can be based on this representation of viscous boundary conditions; this is illustrated in the context of several examples in two dimensions.

BOOTY, Michael (New Jersey Institute of Technology, USA)

Time-dependent fast deflagration waves

A reduced asymptotic model is presented in the limit of small inverse activation energy, $\epsilon \rightarrow 0$, to describe the time-dependent behavior of a class of premixed deflagration waves. The model is similar to the reaction-sheet or flamelet models of combustion but the difference lies in the range of wave propagation Mach numbers considered, and here the initial Mach number M and ϵ satisfy the scaling relation $M = O(\epsilon)$. The reduced model requires numerical solution, and example results are given relevant to deflagration to detonation transition. A similar model for the scaling relation $M = O(1)$ will be presented if time permits.

DOLD, John W (UMIST, UK)

Emergence of a weak detonation in compressible self-ignition

Using the limit of increasing thermal sensitivity, or large activation energy, asymptotic reductions of the model equations for a reactive-Euler fluid will be described. Clarke's equation, which is the reduction that is initially most relevant for detonation initiation via a shock wave, leads to an asymptotic breakdown which matches with an entirely supersonic or "weak" detonation structure, provided such a solution can be found. The analysis of events associated with breakdown of this structure, when the mass-flux falls below a critical "Chapman-Jouget" value, is described in a companion presentation. This is a joint work with A K Kapila.

KAPILA, Ashwani K (Rensselaer Polytechnic Institute, USA)

Rapid transition: From weak detonation to Chapman-Jouguet structure

Recent theoretical analyses, based on large state-sensitivity of the underlying kinetics, have produced an asymptotic picture of the sequence of events that ensue when a homogeneous reactive medium is subjected to a stimulus that makes it detonate. Such a stimulus may, for example, consist of a sufficiently broad, but small-amplitude, hot spot in an otherwise uniform initial state. The scenario then consists of a localized thermal runaway, followed by the appearance of a supersonic reaction wave (effectively, a weak detonation) that decelerates as it advances into the medium. When the wave has slowed down sufficiently, so that a sonic point just appears in the flow behind the wavehead, a relatively rapid transition to a conventional, ZND (Zeldovich, von Neumann, Doering) structure occurs. An asymptotic description of the mechanism for such a transition is the subject of this presentation.



SHORT, Mark (Theoretical and Applied Mechanics, University of Illinois, USA)

Detonation initiation by slowly-varying initial flow non-uniformities

We examine the critical conditions for the initiation of a detonation in a nonuniformly perturbed reactive fluid. Initial perturbations in temperature, pressure and velocity are considered. By assuming a large activation energy and a slow variation of the initial fluid nonuniformities in space, an analytical approximation is obtained for the path of the induction flame arising in Dold and Kapila's theory of detonation initiation. The role of each initial perturbation in defining the path of the flame is explained. We also explain how to rationalize and extend Zeldovich's well-known criteria for detonation initiation. Extensions to three-dimensional geometries are also given.

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ARNOLD, Martin (DLR German Aerospace Centre, Institute of Robotics and System Dynamics, Germany)

Waveform relaxation and the coupled simulation of pantograph and catenary

The dynamical simulation of the interaction between pantograph and catenary at high speeds is a typical example of coupled problems in computational mechanics. The equations of motion are derived in a weak descriptor form that combines partial differential equations describing the catenary dynamics with a differential-algebraic system modelling the pantograph. In the numerical solution methods from multibody dynamics and structural mechanics are coupled by waveform relaxation. We discuss the convergence and the implementation of the waveform relaxation method and illustrate its efficiency by results of numerical tests.

CAMPBELL, Stephen L (North Carolina State University, USA)

PDAEs and DAEs

PDAEs are mixed systems of partial, differential, and algebraic equations. Recently, there has been considerable interest in several areas in working with these systems. The finite dimensional approximations of PDAEs are often DAEs. Several natural questions arise: What is the relationship between the approximating DAE (ADAE) and the PDAE? What advantages and insights are provided in working with PDAEs by using a DAE perspective? Are there technical problems that must be dealt with when working with the ADAEs which occur because they are ADAEs? These and related questions will be discussed.

VÖGEL, Martin (Technische Universität München, Germany)

A virtual test driver for virtual cars

Methods for Virtual Prototyping and Digital Mockup are of vital importance for many automotive manufacturers in order to reduce product development time and cost. Test drives in the computer carried out by numerical simulation of full vehicle dynamics play a key role within these technologies. Using a multi body system model (MBS) handling characteristics of a new car can be examined early in the development process. The dynamical properties of a vehicle can only be rated by investigating the closed loop of driver, vehicle and environment. We are developing a two phase nonlinear position control algorithm for optimal guidance of virtual cars along arbitrary test tracks, which can be used as a virtual test driver.

WINCKLER, Michael J (Interdisciplinary Center for Scientific Computing, University of Heidelberg, Germany)

Optimal control problems in engine design

The optimization of engine components is an important task to improve vehicle performance. One aspect is the optimal control of the valve movement through design of the shape of the cam. An optimization method for this discontinuous multibody system using a multiple-shooting discretization and an SQP-method for optimization is presented. Treatment of discontinuities through switching functions and updates of the gradients in the presence of shocks ensures convergence of the optimal control problem. Extension to optimal design over a variety of working conditions leads to a multiple set-point structure that can be exploited to speed up the computation.

CIARLET, Patrick P, Jr (ENSTA/UMA, France)

Solving numerically the time-dependent Maxwell equations in domains with reentrant corners

When the computational domain is a polygon with reentrant corners, we split up the solution of Maxwell's equations into the sum of a regular part and a singular part. The singular part belongs to a finite dimensional space spanned by the solutions of a steady state problem, whereas the regular part can be approximated by an H^1 -conforming Finite Element Method.

Numerical results will be presented that illustrate the relevance of the decomposition, and comparisons will be made with other approximating techniques, such as the Finite Volume Method.

This is a joint work with Franck Assous and Jacques Segré.

KANGRO, Urve (Tartu University, Estonia)

Singularities of extensions of solutions of Helmholtz's equation

Generally speaking, when one extends a scattered field to the interior of a perfectly conducting scatterer the extension will have one or more singularities. The positions of these singularities are instrumental in determining the rate of convergence of certain integral equation techniques for solving the scattering problem. To use the techniques in question it is best to have prior knowledge of the locations of the singularities. In this talk we will present a solution of this problem and discuss the application to numerical methods.

LOHRENGEL, Stephanie (ENSTA/UMA, France)

How to handle singularities of the electromagnetic field in regions with corners by nodal finite elements

In regular domains, the time-harmonic Maxwell equations allow a discretization by means of nodal finite elements (solve a regularized problem similar to the vector Helmholtz equation). In the vicinity of reentrant corners and edges, the electromagnetic field becomes singular, and a nodal FEM does not approximate in general the solution. Two issues are proposed: The *singular field method* is based on the splitting of the solution into a regular part (treated by nodal finite elements) and a singular part taken into account explicitly. Numerical results illustrate the approach. Secondly, we discuss *penalty methods* with respect to the boundary condition. This is a joint work with Patrick Ciarlet and Christophe Hazard, ENSTA/UMA, France.

RAMDANI, Karim (UMA Laboratory, ENSTA, France)

Singularities of non elliptic transmission problems: Application to the analysis of a superconductive micro-strip line

Finding the guided modes of a superconductive micro-strip line amounts to solve an eigenvalue problem involving an operator A associated to a non elliptic transmission problem. Indeed, in the framework of London's model for superconductivity, the dielectric permittivity takes negative values in the superconductive strip. As a first step for solving this problem, we study here the selfadjointness of the unbounded operator A . Using an integral equation method, we show that if the interface between the dielectric and the superconductive media is regular, A is selfadjoint. If the interface has a corner, the study of the singularities using Mellin transform allows us to derive a necessary and sufficient condition on the contrast between the two media for selfadjointness.

HENROT, Antoine (Ecole des Mines and Institut Elie Cartan, Nancy, France)

Convexity of optimal shapes

In this talk, we present different methods to prove that the solution of some optimal design problem is convex. We will work with the model problem of minimizing capacity with a volume constraint but, of course, the methods we present have a wider scope. The first method consists in proving that the optimal domain must coincide with its convex hull. We prove that by using in a clever way the maximum principle. In the second method (which works only in 2 dimensions), we prove directly that the level sets of the capacity potential are convex. That yields the result since the optimal shape is the level set corresponding to the value 0. The third method (which also works only in 2 dimensions) consists in proving that the curvature of the boundary of the optimal domain has to be positive. We use essentially for that the Hopf's maximum principle. We also show, with another example, that such a condition (positivity of the curvature) can come directly from the optimality conditions.

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HÖMBERG, Dietmar (Weierstrass Institute for Applied Analysis and Stochastics, Germany)
Optimal shape design of inductor coils for surface hardening

Our research is stimulated by the demand for producing components with less weight and higher precision, especially in automotive industry. The underlying mathematical model consists of a vector potential formulation for Maxwell's equations coupled with the energy balance and an ODE to describe the solid-solid phase transition in steel during heating. Depending on the shape of the coil we control the volume fraction of the high temperature phase. Since the coil is modeled as a tube, it can be characterized by its defining curve. We establish well-posedness results for our model, derive optimality conditions and conclude with some preliminary numerical results. This is a joint work with Jan Sokolowski.

JOUVE, François (CMAP, Ecole polytechnique, France)

Eigenfrequency optimization in optimal design

We maximize the first eigenfrequency, or a sum of the first ones, of a bounded domain occupied by two elastic materials with a volume constraint for the most rigid one. A relaxed formulation of this problem is introduced, which allows for composite materials as admissible designs. These composites are obtained by homogenization of fine mixtures of the two original materials. We prove a saddle-point theorem that permits to reduce the full (unknown) set of admissible composite designs to the smaller set of sequential laminates. A numerical algorithm is proposed. Numerical results are presented for various 2d and 3d problems.

This is a joint work with Grégoire Allaire and Sylvie Aubry, LAN, Université P. et M. Curie, Paris.

SOKOLOWSKI, Jan (Institut Elie Cartan, University Henri Poincaré Nancy I, France)

Topological derivative, Part I. Laplace equation

We show that there exists the topological derivative $T(x) = \lim_{\rho \downarrow 0} \frac{J(\Omega \setminus \overline{B_\rho(x)}) - J(\Omega)}{|B_\rho(x)|}$ of the shape functional $J(\Omega)$. $T(x), x \in \Omega$ provides the information on the infinitesimal variation of the shape functional J if a small hole is created at $x \in \Omega$. The results are given for the shape functionals depending on solutions of the Laplace equation in 2D and 3D.

This is a joint work with Antoni Zochowski.

ZOCHOWSKI, Antoni (Systems Research Institute of the Polish Academy of Sciences, Poland)

Topological derivative, Part II. Elasticity system

Given shape functional $I(\rho)(x) = J : \Omega \setminus \overline{B_\rho(x)} \rightarrow R$, defined for sufficiently small ball $B_\rho(x) = \{y \in \mathbb{R}^N \mid \|y - x\| < \rho\}$, $N = 2, 3$, depending on solutions of an elasticity system defined in $\Omega \subset \mathbb{R}^N$. For $N = 2$ the following expansion is obtained $J(\Omega_\rho) = J(\Omega) + \frac{\rho^2}{2} I''(0^+) + o(\rho^2)$ with an explicit form of the function $2\pi T(x) = I''(0^+)(x)$. The topological derivative $T(x), x \in \Omega$, is used for numerical methods of the topology optimization.

This is a joint work with Jan Sokolowski.

HABER, Eldad (University of British Columbia, Canada)

Solution of large scale inverse problems using inexact Krylov-Newton method

Solving large scale nonlinear inverse problem involves with the reconstruction of a model from a discrete set of measurements. In this talk the forward problem is given by a differential equation of the form $A(m)u = f$ where $A(m)$ is the forward modelling operator, m is the model and f is some right hand side. The inverse problem is to find m given the values of u in some discrete locations. Such problems are very ill-posed and solved using Tikhonov regularization. $\min \phi = \|Qu(m) - u^{obs}\|^2 + \beta \|W(m - m_0)\|^2$ where Q is a projection operator and W and m_0 represent our a-priori information. The solution to this nonlinear problem is usually preformed using the Gauss-Newton method. The functional ϕ is linearized and in the k^{th} iteration the problem solved is $\min \phi^{lin} = \|Qu(m_k) + J(m_k)\delta m - u^{obs}\|^2 + \beta \|W(m_k + \delta m - m_0)\|^2$ where $J(m) = \partial Qu(m)/\partial m$ is the sensitivities. The major bottle necks of the solution is the calculation of the sensitivities which is usually a large dense matrix and the inversion of this matrix. This talk will show how to avoid the calculation of the sensitivity matrix and how to effectively invert it and solve the inverse problem. First the sparse representation of J is discussed. It will be shown that in order to calculate a sensitivity matrix-vector product, $J(m)$ does not have to be formed at all. Second, this fact is used in a Krylov-Newton type iteration. Third, the Krylov-Newton method is accelerated by calculating only an approximate matrix-vector product which is regarded as inexact Krylov-Newton method. These concepts are demonstrated on the 3D DC resistivity inverse problem which involves with the recovery of the a conductivity function from the measurements of electric potential on the surface.

HANKE, Martin (Fachbereich 17 Mathematik, Johannes-Gutenberg-Universität Mainz, Germany)

A new method in impedance tomography imaging

Recently, Martin Brühl and the author developed a computational method on the basis of impedance tomography imaging to identify the conductivity coefficient of a body which consists of a number of inclusions in a homogeneous background medium. In this presentation we present theoretical and computational results to discuss limitations of this method and possible extensions to more general applications such as, e.g., the reconstruction of conductivities which are not piecewise constant and the reconstruction of cracks in nondestructive testing.

This is joint work with Martin Brühl and Michael Pidcock.

TAI, Xue-Cheng (Department of Mathematics, University of Bergen, Norway)

Identification of discontinuous coefficients from elliptic problems using total variation regularization

We propose several formulations for recovering discontinuous coefficient of elliptic problems by using total variation (TV) regularization. The motivation for using TV is its well-established ability to recover sharp discontinuities. We employ an augmented Lagrangian variational formulation for solving the output-least-squares inverse problem. In addition to the basic output-least-squares formulation, we introduce two new techniques to handle large observation errors. First, we use a filtering step to remove as much of the observation error as possible. Second, we introduce two extensions of the output-least-squares model; one model employs observations of the gradient of the state variable while the other utilizes the flux. Numerical experiments indicate that the combination of these two techniques enables us to successfully recover discontinuous coefficient even under large observation errors.

This is joint work with Xue-Cheng Tai.

VOGEL, Curtis R (Montana State University, USA)

Multilevel preconditioners for regularized inverse problems

For the numerical solution of large linear systems, the Preconditioned Conjugate Gradient (PCG) algorithm can be very effective if one has a good preconditioner. We will address the construction of effective preconditioners for systems derived from continuous linear operators of the form $K^*K + \alpha L$, where K is compact, L is a diffusion operator, and α is a small positive parameter. We will also evaluate their performance on an example arising in image deblurring (deconvolution).

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BEEVERS, Cliff E (Heriot Watt University, Edinburgh, UK)

The emerging philosophy behind computer based assessment

The computer can play a role in several forms of assessment: diagnostic and self-testing, continuous and grading assessment. Automatic marking has many benefits for the human teacher: it is objective, fast, accurate, flexible and robust. The best test engines expect students to input mathematical expressions as answers much as in a written examination. Over the last decade many HCI issues in mathematical assessment by computer have been resolved. Students highlight as important the issue of partial credit if the computer is to grade their work fairly. This session will concentrate on the educational aspects of an assessment engine for Mathematics.

This is joint work with D J Fiddes, M G McGuire, D G Wild and M A Youngson.

CLEMENTS, Dick R R (University of Bristol, UK)

Essential mathematical concepts needed by users of computer algebra

Computer algebra systems have great potential for professional engineers, scientists and technologists. They can reduce the tedium of routine manipulation required in some mathematical models and procedures, give a greater assurance of accuracy and even enable users to apply techniques which they might find difficult without such assistance. But learning the basic concepts, particularly of the more sophisticated and capable computer algebra systems, is itself a mathematical activity. For instance the formal concepts of functions must be grasped very clearly if the user is to get the best from these systems. This paper will identify and explore some theoretical concepts which may be seen as essential enabling skills for users of computer algebra systems.

CROFT, Anthony C (Loughborough University, UK)

A residual mathematical core for the incorporated engineer

SARTOR3 presents a challenge to designers of mathematics courses for engineers. There is a need to differentiate clearly between the educational experience of prospective chartered and incorporated engineers. The chartered engineer requires a range of higher level mathematical skills whilst the emphasis for incorporated engineers is on the ability to carry out routine mathematical procedures. Many such procedures can be performed using computer algebra systems and it is clear that incorporated engineers should learn to use such systems. In this talk we will discuss what mathematics these students should learn in order to be both intelligent users of technology and effective incorporated engineers.

This is a joint work with D A Lawson & N C Steele.

GOLDFINCH, Judy (Napier University, Edinburgh, UK)

The Sumsman project and its implications for computer-based assessment

Since 1996, four linked Metropolitan Area Networks (MANs) have been available to Scottish HEIs for use in teaching and learning. To stimulate innovative use of the MANs, the Scottish Higher Education Funding Council (SHEFC) supported a small number of subject-based projects within phase 2 of its Use of MANs Initiative (UMI2). The outcomes of one of these projects, Scottish Universities Mathematics and Statistics across the MANs (SUMSMAN), will be described, with particular emphasis on the implementation of computer-based assessment in Mathematics and Statistics. This talk represents the work of the SUMSMAN Project Team.

LABORDE, Colette (Laboratoire Leibniz-IMAG, University Joseph Fourier, Grenoble, France)

Core geometrical knowledge for using the modelling power of geometry with Cabri-geometry

Euclidean geometry has disappeared from some curricula at secondary school and university. This situation may change in the next few years. The power of geometry as a modelling tool, which allows a global representation of a system, is deeply reinforced by the availability of software packages of dynamic geometry such as like Cabri-geometre. Such open ended environments offer a large range of geometrical tools for creating dynamic geometrical figures which can be fully animated. The talk will investigate fundamental geometrical ideas so that the user of such software should be able to develop with linkages into other knowledge domains.

LAWSON, Duncan A (Coventry University, UK)

Formative assessment using CAA

Formative assessment, where students hand in work which tutors return annotated with comments, has been a casualty of the increased pressures on academic staff time. However, this is a valuable part of the learning experience. This talk describes how computer-aided assessment (CAA) can provide a means of preserving formative assessment within the curriculum at a fraction of the time cost involved with written work. CAA no longer means only multiple choice. Sophisticated, yet easy to use, software packages, like Question Mark Designer, permit a variety of assessment styles. The talk will illustrate some of the styles available.

This is a joint work with N C Steele.

MUSTOE, Leslie R (Loughborough University, UK)

How far should the residual core of mathematics be affected by the computer?

Advocates of the increasing use of the computer in the teaching and learning of mathematics claim that certain topics and techniques need no longer be taught because the ready availability of the computer has rendered them obsolete. At the same time, there has been a reduction in the mathematics syllabus at all levels, leading to calls from many quarters that this trend has gone too far and must be reversed. How far should the access to so much computer power influence the core of mathematics which needs teaching at different levels? This paper addresses that question.

SIMS WILLIAMS, Jonathan H (Bristol University, UK)

Open testing with a large databank of multiple choice questions

A major problem of using computer testing is the lack of enough computers to test a whole class simultaneously. Unless all members of the class are tested at the same time, those who do the test later may gain an advantage. If however, we could set a very large number of tests all of the same difficulty and which took about the same time to complete; then we could allow students to take tests in their own time. This paper will discuss attempts to realise this concept at Bristol University.

SUTHERLAND, Rosamund (University of Bristol, Graduate School of Education, UK)

School algebra and the symbol sense of the adult mathematician

For a number of years algebra and other formal aspects of mathematics have been de-emphasised in UK schools. Within this presentation I shall draw on a recent Royal Society report - Algebra Pre-16 - in order to discuss some of the complex reasons for this phenomena. I shall also present ongoing work with undergraduates to highlight the effects that this is having on mathematics-related courses in Higher Education. I shall argue for the need to educate young people to develop confidence and competence with algebra as a means of expressing mathematical ideas and because algebra provides a gateway to mature uses of mathematics, including work with computers.

EWING, Richard E (Institute for Scientific Computation, Texas A&M University, College Station, Texas, USA)

Mathematical modeling and simulation for applications of fluid flow in porous media

This talk will discuss various mathematical models for describing single- and multi-phase, multicomponent fluid flow processes through porous media in reservoir simulation and in subsurface contaminant transport and remediation. Overview of various numerical techniques on these problems will also be given.

LIN, Tao (Department of Math., Virginia Tech., USA)

A non-conformal immersed finite element method for interface problems

We consider a non-conformal finite element method for boundary value problems whose coefficients are discontinuous. The basis functions in this method are constructed as piece-wise linear polynomials that satisfy the jump conditions approximately (or even exactly in certain situations). In addition, the mesh in this method does not have to be aligned with the interface because the interface is allowed to pass through the elements. Therefore structured Cartesian mesh can be used in this method. We will show that this finite element method has a second order convergence rate in L^2 norm, and the usual first order convergence rate in H^1 norm. Representative numerical examples will be provided to illustrate features of this method.

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LYONS, Stephen L (Upstream Strategic Research Center, Mobil Technology Company, Texas, USA)
A family of Eulerian-Lagrangian localized adjoint methods for multi-dimensional advection-reaction equations

In the simulation of some enhanced oil recovery processes or bio-remediation of ground water contaminants, the mass conservation equations are a system of advection dominated advection-reaction equations. To improve the performance of these simulations, we have developed a family of Eulerian-Lagrangian localized adjoint methods for the solution of initial-boundary value problems for first-order advection-reaction equations on general multi-dimensional domains. Different tracking algorithms, including the Euler and Runge-Kutta algorithms, are used. The derived schemes are fully mass conservative and solve advection-reaction equations in a fashion such that the numerical dispersion is essentially eliminated. Moreover, the resulting coefficient matrices of these schemes are regularly structured, well-conditioned, symmetric and positive-definite. Such matrices can be very efficiently solved, for example, the conjugate gradient method using an optimal ordering can be used without any preconditioning. Numerical results are presented to compare the performance of these methods with many well studied and widely used methods, including the upwind finite difference method, the Galerkin and Petrov-Dalerkin finite element methods with backward-Euler or Crank-Nicolson temporal discretization, and the streamline diffusion finite element methods.

QIN, Guan (Upstream Strategic Research Center, Mobil Technology Company, Texas, USA)
Analysis of a compositional model for fluid flow in porous media

In this presentation we consider a compositional model for multicomponent three-phase fluid flow in porous media. The model consists of Darcy's laws for volumetric flow velocities, mass conservation for hydrocarbon components, thermodynamic equilibrium for mass interchange between phases, and an equation of state for saturations. These differential equations and algebraic constraints are rewritten in terms of various formulations of the pressure and component-conservation equations. Phase, weighted fluid, global, and pseudo-global pressure and component-conservation formulations are analyzed. A numerical scheme based on the mixed finite element method for the pressure equation and the Eulerian-Lagrangian localized adjoint method for the component-conservation equations is developed. Numerical results are reported to show the behavior of the solution to the compositional model and to investigate the performance of the proposed numerical scheme.

WANG, Hong (University of South Carolina, Columbia, USA)
An ELLAM-MFEM approximation to miscible displacement in porous media

In this talk we present an accurate and efficient approximation technique to miscible displacement in porous media with point sources and sinks by an Eulerian-Lagrangian localized adjoint method and mixed finite element methods. Numerical Results will be presented to show the strength of the proposed method.

DAUGE, Monique (Universite de Rennes 1, France)
On the Cosserat spectrum in polygons and polyhedra

The Cosserat problem is a classical example that involves finding the spectrum of a non-compact operator. We investigate the cases of clamped and traction-free boundary conditions. We give a full characterization of the essential spectrum. Using asymptotic analysis constructions, we prove the existence of discrete spectrum in rectangles with aspect ratio smaller than 0.47. This is joint work with M. Costabel.

GASTALDI, Lucia (Dipartimento di Matematica, Universita' di Brescia, Italy)
Finite element approximation of eigenproblems in mixed form

It is well-known that the inf-sup and ellipticity in the kernel properties are sufficient conditions in order to have good approximation properties for linear problems in mixed form. Unfortunately the above conditions are not sufficient to give also good approximation properties for eigensolutions. A reason of failure is hidden in the definition of the operator whose spectrum has to be approximated. We intend to enlighten this question, giving a proper definition of such operator so that it is compact. Moreover we introduce some abstract sufficient conditions which imply the convergence of the spectrum. This is a joint work with D Boffi and F Brezzi.

JOLY, Patrick (INRIA, France)

Numerical approximation of spectral problems arising in open waveguide problems

Open waveguides are invariant in some privileged space direction and have an unbounded cross section: an optical fiber for instance. Guided waves propagate along the direction of invariance but have a finite transverse energy. They are eigenvectors of selfadjoint eigenvalue problems for second order elliptic operators in an unbounded 2D domain (the cross section). These operators do not have a compact resolvent : they always have a non empty essential spectrum and possibly eigenvalues. We shall present numerical methods which reduce numerical computations to a bounded subregion via appropriate transparent boundary conditions. The eigenvalues are then characterized as fixed points of eigenvalues of parameterized selfadjoint operators defined in the bounded subregion and having a purely discrete spectrum.

RAPPAZ, Jacques (Ecole Polytechnique Federal de Lausanne, Switzerland)

Spectral pollution in finite element approximations and applications

Galerkin approximations of variationally posed eigenvalue problems without any assumption of compactness usually involve spectral pollution effects in which appears one or several spurious eigenvalues. By using an extension of the notion of essential numerical range of an operator, it is possible to define regions in the complex plane where there is no spurious eigenvalues and where the spectral approximations are stable. In a general framework, we present here a theorem of localization of the region where pollution may occur and we give some examples. In particular, we apply the theory to the membrane approximation of a thin shell (see J Rappaz, J Sanchez Hubert, E Sanchez Palencia and D Vassiliev, *On spectral pollution in the finite element approximation of thin elastic "membrane" shells*, Numer. Math. 75, 473-500 (1997)) in which the vibration problem is associated with a non-compact resolvent operator and spectral pollution could appear when computing Galerkin approximations.

SURI, Manil (University of Maryland, Baltimore County, USA)

On the approximation of the spectra for buckling problems

We consider the linearized buckling model presented by Professor B. Szabó, based on finding the lowest multiple λ_0 of an initial stress σ which causes instability. We show that this λ_0 is the infimum of values λ for which an operator of the form $(A - \lambda B(\sigma))$ fails to have a bounded inverse. Here, A and B are both operators which involve the same order of derivatives on the solution, so that the operator $A^{-1}B$ is non-compact. We discuss convergence of the FEM eigenvalue approximations when the domain is assumed to be thin, and also make some remarks about the non-thin case.

BROOMHEAD, David S (University of Manchester Institute of Science and Technology, UK)

Embedding, oversampling and the estimation of nonlinear channels

There has been a lot of recent interest in the blind estimation of communications channels using oversampling techniques. Generally this work applies to linear, finite impulse response channels. Here we suggest how a corresponding theory may be developed for recursive nonlinear channels. We claim that it is natural to model such channels as iterated function systems, and describe a relevant delay embedding theorem and how it may be applied to the blind estimation problem.

MCLAUGHLIN, Stephen (Dept of Electronics and Electrical Eng, University of Edinburgh, UK)

Nonlinear dynamics in speech synthesis and characterisation

This talk addresses recent suggestions in the literature that the generation of speech is a nonlinear process. This has sparked great interest in the area of nonlinear analysis of speech with a number of studies being conducted to investigate whether low dimensional chaotic attractors exist for speech. This talk examines a corpus of sustained vowel sounds which were recorded for this study to ensure dynamical invariance. The sounds are assessed by a range of the invariant geometric features developed for the analysis of chaotic systems such as correlation dimension, lyapunov exponents and short-term predictability. The results presented suggest that although voiced speech is well characterised by a small number of dimensions it is not necessarily chaotic. Finally, some synthesis techniques, based on nonlinear methods, for voiced sounds are developed.

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PENTEK, Aron (Marine Physical Laboratory of the Scripps Institution of Oceanography University of California, USA)

Nonlinear classification of time series using dynamical models

We discuss the theory and design of automated acoustic detection and classification algorithms based on dynamical systems theory. Specifically, we develop a novel method for the estimation of dynamical signal models, motivated by the Yule-Walker equations of AR modeling theory. We demonstrate that nonlinear dynamical models can simultaneously incorporate linear and nonlinear signal information, but also contain terms which express information about the deterministic signal evolution. Finally, we apply these ideas to the analysis of real-world, broadband sonar recordings, and compare the performance for the dynamical detector with a band-matched energy detector. This is a joint work with Jim Kadtko, Marine Physical Laboratory, and Ron Lennartsson, Swedish Defense Research Establishment (FOA).

ROBINSON, John W C (Natl. Defence Research Est., Sweden)

Information theoretic distance measures in stochastic resonance

We show how some common information theoretic distance measures can be applied to yield alternative definitions of phenomena known under the name stochastic resonance. This yields new insights into the mechanisms underlying these phenomena, provides new methods for analysis, and links the phenomena to fundamental bounds for information processing in nonlinear dynamical systems. This is a joint work with Johan Rung and Daniel Asraf, both at Natl. Def. Res. Est., Sweden.

STARK, Jaroslav (University College London, UK)

A Takens Embedding Theorem for stochastic systems

The analysis of time series obtained from dynamical systems is usually based on delay reconstruction methods. The theoretical justification for these is given by Takens Embedding Theorem. Existing versions of this theorem assume that the time series is generated by an autonomous deterministic system. This is rarely the case in practical applications: most real systems are noisy, and even when the noise can be neglected, many signal processing systems are subject to arbitrary input signals. This talk will describe how to extend the theorem to cover these cases and discuss the implications for the structure of the resulting time series.

FAIRWEATHER, Graeme (Colorado School of Mines, USA)

Alternating direction implicit orthogonal spline collocation methods for initial/boundary value problems

Alternating direction implicit (ADI) techniques, introduced in the context of finite differences for parabolic and elliptic equations by Peaceman and Rachford (1955), have been used extensively over the last four decades in the numerical solution of time-dependent problems. ADI finite element Galerkin methods for parabolic and hyperbolic problems in two space variables were first formulated and analyzed by Douglas and Dupont (1971). By mimicking ADI Galerkin methods, various authors formulated and implemented ADI orthogonal spline collocation (OSC) schemes to solve some practical problems involving parabolic equations. However, no rigorous convergence analyses of ADI OSC schemes were derived until the work of Fernandes and Fairweather (1993). In this paper, we overview recent progress in the development of ADI OSC methods for initial/boundary value problems. In particular, we describe such methods for non-selfadjoint parabolic problems and second order hyperbolic problems which have no finite element Galerkin counterparts, and also discuss the ADI OSC solution of Schrödinger-type problems.

KHALIQ, Abdul Q (Western Illinois University, USA)

Parallel LOD methods for reaction-diffusion systems

Locally One Dimensional (LOD) methods are developed for the reaction-diffusion systems in multi-space dimensions utilizing Strang-like splitting. The non-linear reaction terms are treated in a linearly implicit manner that avoids the necessity of iterating at each time step, while maintaining stability properties of corresponding one-dimensional operator. The elegant methods of Lawson-Morris (1978), and Verwer-de Vries (1985) are couched into this technique and are shown to be computationally efficient. The method based on rational approximants with real distinct poles offers parallelism across the system. Numerical results are presented on reaction-diffusion systems including problems with stiff chemistry and population ecology. This is a joint work with David A Voss.

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TEMAM, Roger (Indiana University, Department of Mathematics, USA)

Some remarks on dynamic multilevel methods

In this lecture we will discuss some aspects of multilevel methods which are based on the splitting of the unknown into arrays of unknowns, including stability analysis and error analysis.

VERWER, Jan G (Center for Mathematics and Computer Science (CWI), The Netherlands)

Results on splitting stiff advection-diffusion-reaction problems

Standard stiff ODE integrators are generally not recommended for the numerical time integration of large scale, stiff systems of 3D advection-diffusion-reaction equations $\frac{\partial c}{\partial t} + \nabla \cdot (\underline{u}c) = \nabla \cdot (K \nabla c) + R(c)$, $c = c(\underline{x}, t)$, $c \in \mathbb{R}^m$, $\underline{u} \in \Omega \subset \mathbb{R}^3$. In particular, when m is large, say up to 100 as for example encountered in air pollution modelling, routinely used solvers applied in a Method of Lines manner would require excessive memory and CPU time. This has led to the use of special time integration techniques, mostly using a form of 'splitting'. Splitting may be used at the operator level, which enables Implicit splitting. Alternatively one may use an implicit-explicit (IMEX) integration formula or an implicit or linearly implicit formula combined with the technique of Approximate Matrix Factorization (AMF). IMEX can be interpreted as splitting within a method. Likewise, AMF can be interpreted as splitting at the level of the numerical algebra computations. In this lecture we discuss results for these various forms of splitting, with emphasis on air pollution applications.

ALFONSO, Giovanni C (Department of Chemistry and Industrial Chemistry, University of Genova, Italy)

Molecular weight effect on crystal nucleation in sheared polymer melts

Polymer processing usually involves mass flow prior to solidification. Macromolecular conformation in flowing melts deviates from the random coil characteristic of quiescent conditions: sequences of chain segments are oriented and elongated in the flow direction. The equilibrium conformation is gradually restored through complex rearrangements when the applied stress is removed. Kinetics of this process can be studied by using the morphological marker of transcrystallinity that develops in systems retaining some level of molecular deformation. The experimental results obtained with several isotactic polybutene-1 samples of different molecular weight will be illustrated and discussed on the basis of current theories. This research has been financed by ASI under contract ARS-96-110.

BONILLA, Luis L (Escuela Politecnica Superior, Universidad Carlos III Madrid, Spain)

Kinetic theory of aggregation and growth in polymers

We propose a kinetic description of the processes of polymer nucleation and growth. The effects of temperature gradients on the nucleation rate are analyzed within a Fokker-Planck type description. This is a joint work with A Revuelta, Escuela Politecnica Superior, Universidad Carlos III, Departamento Matematica Aplicada, Madrid; D. Reguera and J.M. Rubi, Dept. Fisica Fonamental, Facultad de Fisica, Universidad Barcelona.

BURGER, Martin (Industrial Mathematics Institute, University of Linz, Austria)

Modelling multi-dimensional crystallization of polymers in interaction with heat transfer

Mathematical modelling of spatially heterogenous crystallization processes enforces knowledge about the growth of nuclei in heterogenous fields, which may be generated e.g. by the heat transfer process occurring in the polymeric material. We derive a growth model for polymeric crystals based on an experimentally verified assumption. Furthermore we show that the Avrami-Kolmogorov theory for the derivation of kinetic equations on a macroscopic scale is applicable in a very general setup. We deduce an initial-boundary problem for a coupled system of nonlinear PDEs as the kinetic equations of a process with thermal heterogeneities. Finally, the problem of identifying relevant physical parameters from measurable data will be considered. This is a joint work with Vincenzo Capasso, Dept. of Mathematics, University of Milan and Claudia Salani, Dept. of Mathematics, University of Milan.

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EDER, Gerhard (Institute of Chemistry, Linz University, Austria)

Morphological characteristics in the modelling of crystallization kinetics

For the prediction of mechanical properties of a crystallized material one needs knowledge about some of its morphological characteristics. Most of the mathematical models for the description of the kinetics of crystallization used so far in simulation can not be employed, since no morphological quantities show up in the corresponding equations. The classical Kolmogoroff theory contains (implicitly) all the desired structural information for the case of spherulitic crystallization. Using the Steiner formulae from integral geometry one gets important quantities like the contact interface density or the final edge length density of impinged crystallites, which are important for the description of the spreading of forces in a crystallized sample under external load.

GRAMBERG, Heike J J (Eindhoven University of Technology, The Netherlands)

Instabilities in industrial processes for polymer products.

Industrial processes for polymers like: extrusion, fiber spinning, cable coating, or injection moulding, all show specific types of flow distortions. Typical examples are sharkskin or spurt in extrusion, diamond shaped sharkskin in cable coating, front distortions in injection moulding, or spin instabilities. The diamond shaped distortions observed in cable coating seem to be due to exit effects combined with slip. A first trend is rendered by a linearised analysis. Front distortions in injection moulding can be caused by interactions between the velocity field and the temperature. Possibly, they are introduced by temperature differences between the polymeric melt and the wall. This is a joint work with A A F van de Ven.

MANCINI, Alberto (Dip. di Matematica "F.Enriques", Milano, Italy)

Isobaric solidification processes of molten polymers

The determination of P-V-T diagrams for polymers is based on a careful experimental procedure consisting in monitoring the temperature field, the spatial distribution of crystalline volume fraction and the volume of a polymer sample during a cooling process in a series of experiments performed at different values of pressure. A mathematical model has been formulated, including the flow induced by density variations associated to thermal contraction and crystal growth. Numerical computations performed on the model have pointed out relevant features of the process, leading to some interesting physical conclusions. Existence and uniqueness of the solution to the corresponding free boundary problem has been proved. This is a joint work with Antonio Fasano and Salvatore Mazzullo.

MICHELETTI, Alessandra (MIRIAM, Dept. Of Mathematics, University of Milan, Italy)

Boolean models and spatial statistics applied to the modelling of polymer crystallization

A random closed set (RACS) Ξ is a random variable assuming values in the family F of closed subsets of \mathbf{R}^d , equipped with a suitable σ -algebra. A particular type of RACS, very used in applications, is the so called Boolean model, defined by $\Xi = \bigcup_{x_i \in \phi} \Xi_i \oplus x_i$, where $\phi = \{x_i\}_{i \in \mathbf{N}}$ is a point process in \mathbf{R}^d (whose elements are called germs), $\{\Xi_n\}_{n \in \mathbf{N}}$ is a family of RACS (called grains) and \oplus denotes the Minkowski addition. When the sets are spheres of random radius, the Boolean model is a good representation of many real phenomena, like, for example, the morphological structure of polymer crystallization processes. Many real processes often generate geometrical shapes with very strong spatial anisotropies, which may so be approximated by inhomogeneous Boolean models. In this lecture we will provide a review of the main statistical techniques and open problems related to this kind of Boolean Models.

This is a joint work with Vincenzo Capasso, MIRIAM, Dept. of Mathematics, University of Milan, Italy.

SALANI, Claudia (Department of Mathematics, Milano, Italy)

Interaction of the crystallization process of Polymers with temperature field

The development of crystallization is schematized in two steps: birth of nuclei (germs) and growth of crystals. The local crystallinity can be thought as the probability of capture of a certain point by the crystalline phase. So concepts from stochastic geometry are used which include the so called causal cone. The classical Avrami-Kolmogorov formula is revisited in this more general framework.

The crystallization process is strictly connected with the temperature history during the cooling time. Indeed both the nucleation process and the growth of spherulites are dependent upon local temperature and, on the other side, the latent heat of crystallization influences the thermal field via enthalpy.

We describe the coupling of the local temperature with the crystallization process by an hybrid model and by a many-particle model (totally stochastic).

VAN DE VEN, Alfons A F (Eindhoven University of Technology, The Netherlands)

Morphology of polymer blends

The production process of a polymer blend, i.e. a mixture of two or more polymers, takes place in an extruder. During this process, due to shear stresses, long threads of dispersed phase are formed. Surface stresses can cause these threads to break up in spherical droplets ('Rayleigh instability'). In a blend, interactions between two or more threads are essential. A blend containing two parallel threads is modelled, and the (in)stability of it is investigated. It turns out that both breaking-up in-phase as well as in anti-phase can occur. This is in correspondence with observed experimental results.

This is a joint work with Gunawan A Y, Eindhoven University of Technology, The Netherlands.

ARO, Colin J (Lawrence Livermore National Laboratory, USA)

Implicit hydrodynamics simulation in ALE3D

We will present an overview of the ASCII code ALE3D. ALE3D is a three dimensional unstructured finite element code with arbitrary connectivity, explicit/implicit hydrodynamics with slide surfaces (contact algorithms), chemistry, material strength models, and thermal diffusion. The applications include a variety of manufacturing problems and high explosive safety problems. The linear systems arise in the implicit hydrodynamics and in the thermal diffusion package. We will discuss the structure of the matrices and our experiences of solving them with direct and iterative methods. This is joint work with Juliana J Hsu.

CHOW, Edmond (Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, USA)

Implicit solution methods for multiphysics computations with sliding surfaces

We describe the linear algebraic equations that arise from the implicit simulation of solid-fluid interactions when sliding surfaces are modeled. Additional impenetrability conditions match the normal displacements on both sides of a slide surface. Experimentally, these additional equations make the global set of equations much more difficult to solve. We describe various preconditioning techniques for the iterative solution of these equations. The preconditioners approximate the block of equations on each side of the slide surface and use reduction techniques to eliminate the slide surface equations either exactly or inexactly. Numerical experiments are used to gain insight into the method and its effectiveness.

FARHAT, Charbel (University of Colorado, Boulder, USA)

High-resolution and high performance implicit aeroelastic and acoustoelastic computations

We present a computational framework for the high-performance simulation at high resolution of coupled fluid/structure problems pertaining to the fields of aeroelasticity and acoustoelasticity. This computational framework includes, among others, a methodology for higher-order space/time accurate implicit viscous CFD computations on unstructured moving grids, a robust spring analogy method for updating dynamic meshes, a conservative scheme for exchanging aerodynamic, elastodynamic, and acoustic data across non-matching fluid/structure interfaces, a second-order time-accurate implicit staggered procedure for solving the two-way coupled fluid/structure equations of motion, and fast domain decomposition based iterative solvers. We discuss some parallel implementation aspects of our simulation capability on massively parallel processors, and report on its application to the flutter prediction of wings, the simulation of high-G maneuvers of complete fighter configurations, and the sensitivity analysis with respect to scattering data of acoustic fields scattered by submarine structures. We also present numerical/experimental correlations for some of these problems.

BALL, John M (University of Oxford, UK)

Global attractors for the 3D incompressible Navier-Stokes equations

It is shown that a global attractor in L^2 exists for the 3D incompressible Navier-Stokes equations in a bounded domain under the (unproved) hypothesis that all weak solutions satisfying an energy inequality are continuous from $(0, \infty)$ to L^2 . The analysis is based on a theory of semiflows having possible nonunique solutions, and on use of the energy inequality to deduce strong convergence from weak convergence.

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CHEN, Gui-Qiang (Northwestern University, USA)

Existence, compactness, and asymptotic behavior of entropy solutions

In this talk we will discuss some ideas, approaches, and methods developed recently and study the existence, compactness, and large-time behavior of weak entropy solutions without locally bounded variation, as well as the asymptotic stability of Riemann waves under large $L^1 \cap L^\infty$ or $L^1 \cap BV$ initial perturbations, for nonlinear hyperbolic conservation laws and related equations. Relations between the asymptotic problems and other topics will be addressed including: (a) compactness of weak entropy solution operators; (b) uniqueness of Riemann solutions in the class of L^∞ or BV solutions; (c) singular limits; (d) theory of divergence-measure fields. Some recent results on the compressible Euler equations with general pressure laws as well as geometric structure, and related nonlinear equations will be discussed.

FREISTÜHLER, Heinrich (RWTH Aachen, Germany)

Stability and instability of viscous and inviscid shock waves in one or several space dimensions

Both the large-time stability of viscous shock waves and the spontaneous stability of inviscid shock waves are studied, using the various old and more recent techniques. Particular attention will be given to the stability of undercompressive shock fronts and to a transition from stability to instability occurring for certain families of shock waves that do satisfy Lax's entropy condition.

HOLDEN, Helge (Norwegian University of Science and Technology, Norway)

Operator splitting and the generalized KdV equation

We apply the method of operator splitting to the generalized Korteweg-de Vries (KdV) equation $u_t + f(u)_x + u_{xxx} = 0$ by solving the nonlinear conservation law $u_t + f(u)_x = 0$ and the linear dispersive equation $u_t + u_{xxx} = 0$ sequentially, and analyze the method numerically.

NATALINI, Roberto (Istituto per le Applicazioni del Calcolo, CNR, Italy)

The Barenblatt non-equilibrium model for secondary oil recovery

We present some results about global existence and uniqueness of BV solutions to a quasilinear Goursat problem, which was proposed by G.I. Barenblatt as a singular perturbation of the classical Buckley-Leverett. This model arises to describe two phase fluid flow in permeable porous media, with a special attention to secondary oil recovery, when non-equilibrium phenomena caused by a saturation change are not negligible. Unfortunately this new problem is no more strictly hyperbolic on the boundary of the physical range of the unknown and it is possible to show example where global solutions to the problem do not exist. However for initial data which verify a physical admissibility condition, it is possible to prove existence and stability of solutions. In this case, when the equilibrium relaxation time tends to zero, the sequence of solutions is shown to converge to the entropy solution of the corresponding initial-boundary value problem for the unperturbed Buckley-Leverett equation.

SERRE, Denis A G (Ecole Normale Supérieure de Lyon, France)

On the multi-D stability of some large planar shock waves

Planar Lax shock waves are stable under 1-d perturbations, except in the case where the jump belongs to the space spanned by the outgoing modes. This special case may only concern large shocks for strict hyperbolic systems. However it holds for MHD and in the so-called cubic model. We investigate the multi-d stability of nearby shocks. The results depend upon the dimension d .

SHELUKHIN, Vladimir (Lavrentyev Institute of Hydrodynamics, Russia)

Boundary layer for the compressible Navier-Stokes equations

A mathematical basis for the boundary layer theory is discussed. Particularly, we show that there exists a boundary layer thickness function $\delta(\mu) \downarrow 0$, such that $\delta/\mu^{1/4} \rightarrow \infty$, as $\mu \downarrow 0$, where μ is the vanishing shear viscosity. To this end, we first prove the global unique solvability for the Navier-Stokes equations describing spiral one-dimensional flows of a compressible isentropic fluid between two coaxial circular cylinders. Next, we justify the passage to limit $\mu \rightarrow 0$. Then, we obtain an estimate for the boundary layer thickness matching the above property.

TRIVISA, Konstantina (Northwestern University, USA)

Global discontinuous solutions of the Navier-Stokes equations for compressible reacting flow

Existence theorems are established for global discontinuous solutions to the compressible Navier-Stokes equations for a reacting mixture with discontinuous initial data, which describes dynamic combustion. Uniqueness and qualitative behavior of the discontinuous solutions are discussed. Our approach is to combine the difference approximation techniques with the energy methods and total variation estimates to deal with jump discontinuities. This is joint work with Gui Qiang Chen and David Hoff.

TZAVARAS, Athanasios E (University of Wisconsin-Madison, USA)

On various approximations of the nonlinear wave equation

The nonlinear wave equation is the simplest model of a system of conservation laws. In this talk we review convergence results on approximating weak solutions of the nonlinear wave equation via a variety of approximating mechanisms: first via viscosity, then via relaxation and semi-discrete relaxation schemes, and last via the method of time-step discretization.

WANG, Dehua (University of California, Santa Barbara, USA)

Nonlinear magnetohydrodynamics

The large time properties of solutions to nonlinear compressible magnetohydrodynamics are considered. The initial data are smooth and arbitrarily large. It is proved that the solution will be smooth globally in time. The existence of global solution is established with novel estimates. The pointwise large time limiting behavior of the solution is obtained. This is joint work with Gui-Qiang Chen.

ALPERT, Bradley K (National Institute of Standards and Technology, USA)

Rapid evaluation of exact nonreflecting boundary conditions

The exact nonreflecting boundary conditions for the wave equation and Maxwell's equations - well-known to be nonlocal in both space and time - can be expressed as a convolution of the solution at the boundary from the time of quiescence to the present. These boundary conditions, derived by separation of variables in Cartesian, cylindrical, and spherical coordinate systems, appear to require extensive history of the solution on the boundary. We show, however, that by appropriate representation of the convolution kernels, the history can be reduced to order $O(n \log n)$, where n is the number of points in the discretization of the boundary. This reduction leads to efficient evaluation of the boundary conditions. We present the method and our numerical results.

This is joint work with Leslie Greengard and Thomas Hagstrom.

BECACHE, Eliane (INRIA-Rocquencourt, France)

Application of the fictitious domain to elastic waves

We present a numerical method for solving the diffraction of transient elastic waves by cracks of arbitrary shapes in complex media. To get an efficient method, we want to use regular meshes and at the same time respect the geometry of the crack. This is possible thanks to the fictitious domain method, which takes into account the boundary condition via a Lagrange multiplier defined on the crack. This allows to work with a uniform mesh in the whole domain and an independent mesh on the crack. To do so, we have to consider the free surface boundary condition as an equality constraint, and this leads to the mixed velocity-stress formulation for elastodynamics. At this stage, we want to avoid the inversion of a mass matrix at each time step: we have constructed an original mixed finite element for the velocity-stress formulation leading to an explicit time discretisation scheme (mass lumping). This is a joint work with C Tsogka and P Joly.

GOODRICH, John W (NASA Glen Research Center, Cleveland Ohio, USA)

Hermite methods for hyperbolic systems

A methodology is presented for developing highly accurate finite difference algorithms for evolution equations. The algorithms are local, single step, explicit methods. Realizations that use Hermite spatial interpolation have spectral like accuracy. Examples are shown up to fifteenth order accurate in both space and time. Applications will be to the linearized Euler equations, the Euler equations, and the viscous Burgers equation, in one or two space dimensions. High accuracy and resolution provide for accurate solutions over very long times with modest grid densities, and improve computational efficiency by orders of magnitude over conventional finite difference methods. These methods are highly scalable for parallel architectures.

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HAGSTROM, Thomas (University of New Mexico, New Mexico, USA)

From integral formulas to numerical methods for solving the wave equation

Poisson's integral representation of the solution of the initial value problem is a classical cornerstone of the theory of the wave equation. However, it has not had much application to its numerical analysis. This is due, in part, to the presence of surface integrals. Here we consider reformulations of Poisson's integral in terms of volume integrals of the Laplacian. Discretization of these formulas leads to conservative time-stepping methods of any order of accuracy, with the advantages of flexibility in treating irregular cells enjoyed by numerical integration techniques. In this talk we discuss our still preliminary theoretical and experimental results with these methods.

HESTHAVEN, Jan S (Division of Applied Mathematics, Brown University, Providence, USA)

Fast stable spectral methods on unstructured grids

We discuss the development of fast, stable and accurate spectral methods on generally unstructured nodal sets within the n -simplex. Using truly multi-dimensional Lagrange polynomials we first address the construction of nodal sets for interpolation and resolve this issue through an electrostatic approach. The construction of stable methods on almost general nodal distributions is addressed by showing how to imposing the boundary conditions only weakly through a penalty term. A critical concern of the unstructured methods relates to fast computation of the nodal derivatives. We show how to exploit various symmetries in the nodal sets resulting in a competitive computational framework.

LEVEQUE, Randall J (University of Washington, USA)

High-resolution methods for wave propagation in random media

High-resolution multi-dimensional finite-volume methods for nonlinear conservation laws and other hyperbolic systems have been developed and implemented in the software package CLAWPACK. These methods have recently been applied to acoustics and elasticity problems with discontinuous and rapidly-varying material parameters. The solution of the "Riemann problem" at cell interfaces provides an accurate resolution of waves into reflected and transmitted parts at discontinuities, and the resulting methods can give accurate numerical solutions even in random media. These methods may also serve as a useful tool in testing and comparing homogenization theories.

RADVOGIN, Yulian B (Keldysh Institute of Applied Mathematics, Moscow, Russia)

The characteristic surfaces method for constructing transparent boundary conditions in the nonseparable variables case

The wave equation in unbounded domain is considered. The initial data are to be compact supported. The problem is how to make good use this information. The most methods of constructing transparent conditions on artificial boundaries deal with the separable variable case. The proper technique provides non-local TBC for each mode. Another approach is based on the well-known Kirchhoff method that demands the constancy of coefficients. The presented approach can be briefly described as follows. To solve the original problem numerically outside the artificial boundary one can use the characteristic surfaces as coordinate surfaces $t = \text{const}$. Because the solution on these surfaces is simply structured a moderate number of grid points is needed to approximate this solution up to required accuracy. It can be shown that this characteristic problem is well posed. This method is applied to for the wave equation $u_{tt} = (c^2(y)u_x)_x + (c^2(y)u_y)_y$ in a plane channel $y = \pm 1$.

AREGBA-DRIOLLET, Denise (Mathématiques Appliquées de Bordeaux, Université Bordeaux 1, France)

Some kinetic type schemes for gas dynamics

In the past few years, kinetic models as well as relaxation ones have been used to propose simple, Riemann solver-less numerical schemes for systems of conservation laws. In this talk we adopt the viewpoint of (D Aregba-Driollet and R Natalini, *Discrete kinetic schemes for multidimensional conservation laws*, 1998, submitted) and apply these ideas to some problems related to fluid dynamics. We study the construction of approximations which insure conservation of certain physical properties of solutions and have correct qualitative behaviour. Numerical experiments are presented.

This is a joint work with Vuk Milisic, Université Bordeaux 1, Talence, France and Roberto Natalini, IAC, Consiglio Nazionale delle Ricerche, Roma, Italia.

GUARGUAGLINI, Francesca R (Dipartimento di Matematica Pura e Applicata, Università degli Studi dell'Aquila, Italy)

A kinetic hyperbolic approximation to quasilinear diffusion problems

We present a new discrete kinetic approximation for the Cauchy problem for equations with nonlinear diffusion and convection of the form $\partial_t u + \partial_x A(u) = \partial_{xx} B(u)$, $B' \geq 0$. For this purpose we introduce a class of BGK models with discrete velocities and a double scaling. Let $N \geq 2$ be fixed and let $F^\varepsilon = (f_1^\varepsilon, \dots, f_N^\varepsilon) : \mathbf{R} \times \mathbf{R}_+ \rightarrow \mathbf{R}^N$ be a solution of the semilinear hyperbolic system $\partial_t f_i^\varepsilon + (\lambda_i + \frac{\partial_i}{\sqrt{\varepsilon}}) \partial_x f_i^\varepsilon = \frac{1}{\varepsilon} (M_i^\varepsilon(u^\varepsilon) - f_i^\varepsilon)$, for $i = 1, \dots, N$, and $\varepsilon > 0$. In a paper in collaboration with R. Natalini we show, under suitable consistency assumptions on the function M , the convergence of this approximation to a weak solution to the Cauchy problem as $\varepsilon \rightarrow 0+$. Similar results are also proved in the multidimensional case. Numerical schemes are investigated and their convergence has been proved in a joint work with R Natalini and S Tang.

SERRE, Denis A G (Ecole Normale Supérieure de Lyon, France)

The stability and convergence of semi-linear relaxation

The semi-linear relaxation of a system of N conservation laws $u_t + f(u)_x = 0$ is the approximation through a system of $2N$ balance laws: $u_t + v_x = 0$, $v_t + a^2 u_x = (f(u) - v)/\tau$. Here, $\tau \ll 1$ is a relaxation time whereas a is an a priori chosen velocity. The latter has to satisfy the well-known sub-characteristic condition. We show that the same assumptions than those involved by R. DiPerna in the vanishing viscosity method ensure the stability and convergence as $\tau \rightarrow 0+$.

TZAVARAS, Athanasios E (University of Wisconsin-Madison, USA)

On the kinetic formulation of 2×2 systems of conservation laws

The kinetic formulation of systems of conservation laws is a way of describing a notion of entropy weak solutions that has its origin in ideas from the kinetic theory of gases. At a technical level it requires the calculation of the fundamental solution for the equations describing the entropy structure of the system, and a characterization of the generators of convex entropies. We will describe how this is done for strictly hyperbolic 2×2 systems, and exhibit a kinetic formulation for the equations describing one-dimensional isothermal motions of elastic materials. This is a joint work with B Perthame, ENS-Ulm.

ANDERSON, Alexander A R (University of Dundee, UK)

Continuous and discrete mathematical models of tumour angiogenesis

Tumour angiogenesis is the formation of blood vessels from a pre-existing vasculature in response to chemical stimuli (tumour angiogenic factors, TAF) provided by the tumour, in order to facilitate further tumour growth and invasion. In this talk we present both continuous and discrete mathematical models which describe the formation of the blood vessel network in response to TAF supplied by a solid tumour. The models also take into account essential vessel-extracellular matrix interactions. The theoretical angiogenic networks generated by computer simulations of the discrete model are compared with those observed in *in vivo* experiments.

BELLOMO, Nicola (Dip. Matematica, Politecnico di Torino, Italy)

Tumour-immune system competition: From cellular to continuum theories

The first part of the talk will deal with kinetic modelling of the cellular dynamics of tumours interacting with an active immune defence system in the presence of cytokine signals. The second part will then consider the passage to macroscopic models developed in the framework of multiphase systems. These models are able to describe as a free boundary value problem the evolution of tumour growth during the avascular and the angiogenic phase with formation of necrotic regions, the control of mitosis by inhibitory factors, the angiogenesis process with proliferation of capillaries just outside the tumor surface with penetration of capillary sprouts inside the tumor and the regression of the capillary network induced by the tumor when angiogenesis is controlled or inhibited.

BYRNE, Helen M (School of Mathematical Sciences, University of Nottingham, UK)

Modelling the effect of mutations in solid tumour growth

In this presentation mathematical models will be developed and used to investigate the advantages that cell mutations confer on avascular tumours. Attention will focus on the tumour suppressor gene p53 since this gene is known to play a pivotal role in tumour progression and is present in mutant form in at least 50% containing normal and mutant cells it will be possible to identify those factors which are responsible for the mutant cell population becoming dominant.

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CAMERON, David A (Department of Oncology, University of Edinburgh, UK)

Clinical aspects of modelling cancer growth

Extrapolation of a Gompertz curve fitted to xenograft tumour volumes accurately predicts growth for 7 - 14 days. The tamoxifen-induced deviation from predicted growth correlates with the ratio between apoptosis and proliferation; and in static tumours this permits an estimate of the relative duration of mitosis and apoptosis. In clinical tumours, the advantage of Gompertzian models over others is less convincing than in tumour spheroids or xenografts, partly because of the narrow range of clinically available data on tumour volumes. However published and unpublished data on the applicability of growth models to clinical data will be presented.

CHAPLAIN, Mark A J (University of Dundee, UK)

Continuous and discrete models of tumour cell invasion

Once a solid tumour has acquired its own blood supply vascular tumour growth occurs and cells degrade and invade the surrounding tissue. We present continuous (nonlinear PDEs) and discrete (biased random walk) models of invasion of tissue by tumour cells. Numerical solutions in both one and two space dimensions will be presented and the link between microscopic and macroscopic dynamics will be discussed. The aims of this talk are to show how the tissue matrix governs and modulates (via haptotaxis) the migration of tumour cells and how this may aid us in making predictions about the cells' metastatic ability.

KING, John R (University of Nottingham, UK)

Mathematical modelling of avascular tumour growth

Recent work with JP Ward on the modelling of the growth of avascular tumours will be described. The model predicts the spatial heterogeneity and temporal behaviour observed in multi-cell spheroids; a bifurcation analysis of the large-time behaviour clarifies the conditions under which growth saturation is predicted and those under which continued growth takes place. The results of coupling a model for drug delivery to the one for tumour growth will also be outlined.

PANETTA, John C (Penn State Erie, The Behrend College, USA)

Mathematical modelling of cell-cycle-specific chemotherapeutic drug regimens for cancer

The combination of platinum and Taxol is currently the standard first line chemotherapy for epithelial ovarian cancer. We have developed a mathematical model to help answer several questions about the sequencing of these two drugs. 1.) Does the sequencing of the drugs depend on the cell-cycle and/or pharmacokinetics/pharmacodynamics? 2.) What sequencing does the model suggest is best? 3.) How do the model results compare with current in vitro and clinical studies on delivering this combination of drugs? Like the experimental data the model shows that Taxol before Cisplatin is the better sequence.

PETTET, Graeme J (Queensland University of Technology, Brisbane, Australia)

Cell migration in multicellular spheroids

Multicell spheroids, small spherical clusters of cancer cells, grow until they reach a dormant state where they exhibit a grossly static multi-layered structure. However, at a cellular level the spheroid is demonstrably dynamic with cells migrating from the outer well-nourished region of the spheroid toward the necrotic central core. A consolidation type model for the development of this multi-layered structure, with slow viscous flow of the cells and porous media flow of extracellular water is considered. Crucially, cell motion is determined by the forces generated by cell-cell and cell-matrix interaction and cell proliferation.

SHERRATT, Jonathan A (Dept of Mathematics, Heriot-Watt University, Edinburgh, UK)

Mathematical modelling of tumour invasion: Basic mechanisms and therapeutic implications

Tumour invasion is the process in which cells migrate away from a primary tumour into surrounding tissue, and is a key step in the metastatic cascade. I will describe a mathematical model that addresses the way in which the cells interact with the extracellular matrix surrounding them in an invasive tumour. In particular, I will use the model to show that the pro-invasive pull of extra-cellular matrix is balanced by an anti-invasive pull of the products of matrix degradation. Mathematically, this is represented by a system of mixed hyperbolic parabolic conservation equations, in which solutions of the travelling wave type representing invasion have a novel wave speed selection rule. I will discuss these mathematical results and their biological implications.

SLEEMAN, Brian (School of Mathematics, University of Leeds, UK)

Mathematical models of tumour angiogenesis and the role of angiostatin

In this paper a mathematical model is developed to describe the initiation of capillary formation in tumour angiogenesis. The model includes haptotactic saturation of fibronectin and the role of pericytes and macrophages in regulating angiogenesis. The presence of anti-angiogenic (angiostatin) factors is also considered. It is shown that angiostatins can inhibit capillary growth and demonstrates the possibility of preventing capillary migration in the ECM. The model is based on the theory of reinforced random walks and Michaelis-Menten kinetics.

MUELLER, Jennifer L (Rensselaer Polytechnic Institute, USA)

A reconstruction algorithm for EIT data collected on rectangular electrode arrays

A 3-D reconstruction algorithm in electrical impedance imaging is presented for determining the conductivity distribution beneath the surface of a medium given surface voltage data measured on a rectangular array of electrodes. Such an electrode configuration may be desirable for using EIT to detect tumors in the human breast. The algorithm is based on linearizing the conductivity about a constant value. Reconstructions are presented from numerical and experimental tank data and a sequence of human cardiac data. This is a joint work with David Isaacson and Jonathan Newell.

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GELB, Anne (Arizona State University, USA)

The enhanced spectral viscosity numerical method applied to climatology models

We introduce a new numerical method that stabilizes numerical forecasting models while retaining all of the information necessary to recover a highly accurate solution without Gibbs oscillations. The method consists of first applying the spectral viscosity method to the model, then employing the recently developed enhanced edge detectors to identify the edges of the discontinuities in the solution, and finally post-processing to obtain a spectrally accurate solution. We note that since the edge detection and removal of the Gibbs oscillations occur only in the post-processing step, minimal cost is added to the status quo spectral simulations.

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NIKIFORAKIS, Nikolaos (DAMTP, UK)

Riemann problem based methods and adaptive mesh refinement for global atmospheric modelling

A model for global atmospheric simulations is presented which uses Riemann problem based methods to discretise the governing equations, and adaptive mesh refinement (AMR) for space discretisation. The model is validated using problems with exact solutions; operational evaluation is performed comparing model output against meteorological analyses. The numerical method used provides very accurate results at a low computational cost. AMR enables us to capture a broad range of flow features in an efficient manner. These attributes are demonstrated using case-studies from the evolution of the polar stratospheric vortices and stratosphere-troposphere exchange.

PROVENZALE, Antonello (ICG-CNR, Italy)

Predictability and prediction from time series

In this talk I address the problem of quantifying predictability and making predictions of the future behavior of a system based on the analysis of a recorded time series. In particular, I consider the case of coupled systems with different time scales and of driven systems undergoing on-off intermittency. A Random Analogue Predictor (RAP) is used to make ensemble predictions and to assess the probability of extreme events. The application to the study of long precipitation time series is considered.

ZAVATARELLI, Marco (IMGA-CNR, Italy)

Ecological modelling of the Adriatic sea: Coupling physics with biology

An ecosystem model has been developed by coupling on line the Princeton Ocean Model (POM) with the European Regional Seas Ecosystem Model (ERSEM). The POM/ERSEM system has been implemented in the Adriatic Sea in order to study its ecosystem dynamics. Simulations have been carried out by developing different and increasingly complex (from 1D to high resolution 3D) model set-up. One dimensional simulations concerned the northern Adriatic Basin; The model results highlighted the yearly phytoplankton cycle and its relations with the external nutrient inputs, the seasonal mixing processes and light distribution in the water column. As an intermediate step toward the 3D high resolution application, a coarse resolution 3D implementation with idealized basin geometry was developed. The model results relative to phytoplankton distribution are in good agreement with CZCS climatological satellite pictures of pigment distribution in the basin. Finally, experiments with an high resolution implementation show a more detailed temporal and spatial variability of the biogeochemical properties distribution, furtherly emphasizing the importance of the circulation features in determining such variability.

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CARLE, Alan (Rice University, Houston, USA)

Not entirely automatic differentiation (Part II)

The ADIFOR 2.0 automatic differentiation system makes it possible to augment compute codes to compute accurate derivatives using very little human effort. Getting good performance for some applications, however, requires users of automatic differentiation tools to make a larger investment in time. In this talk I will describe the efforts that have gone into developing an industrial strength sensitivity-enhanced computational fluid dynamics implementation using automatic differentiation. This is joint work with Christian Bischof.

HAMMARLING, Sven (NAG Ltd, UK)

James Hardy Wilkinson and numerical software

The Wilkinson Prize for Numerical Software was established in honour of the outstanding contributions to the field by James Hardy Wilkinson. In this talk we shall review those contributions, together with the influence that Wilkinson had on the development of numerical software. We shall begin by looking at the experiences that influenced Wilkinson himself, look at Wilkinson's own contributions and software developments that directly benefited from his interest, and conclude by trying to assess the effect that Wilkinson has had on numerical software development.

PETZOLD, Linda (University of California, Santa Barbara, USA)

Algorithms and software for sensitivity analysis and optimal control of differential-algebraic systems

Sensitivity analysis and optimal control of large-scale differential-algebraic equation (DAE) systems are challenging computational problems with many important applications. Research issues for algorithms and software include handling of equality and inequality constraints, consistent initialization of DAEs and sensitivities, exploiting structure from the DAE in the optimization, dealing with scaling and ill-conditioning, effective use of automatic differentiation, parallelization and design of user interfaces and application development environments for complex collections of interdependent software. We will briefly describe our progress and experience to date.

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COTSAFTIS, Michel (LTME/ECE, France)

Exact vs asymptotic representation of solution of dynamical equations

Base representations used for differential equations are not adapted for time dependent ones because once the base is fixed the manifold of the solutions may escape from it and be poorly described with spillover effect. Alternative way is to construct the solution with the constraint that power flow is approximated to within prescribed order for a given time interval leading to asymptotic approximation type approach easily developable when small parameter exists in the problem. It is shown that some useful properties of representation are valid independent of parameter value and allow to give exact structure solution very useful for solution analysis and calculation.

MURATA, Junichi (Kyushu University, Japan)

Neural network structure design using genetic algorithm

A Neural Network structure designing method is proposed based on Genetic Algorithms (GA). A new structure coding with a control parameter is devised so that a single chromosome represents not a single but a family of network structures. Thus relevant optimization gives us a chromosome that provides a family of network structures suitable for a set of tasks. Due to this *controllable one-to-many decoding*, we obtain a new good network structure, when we face a new but related task, by only adjusting the control parameter without re-running the GA.

This is a joint work with Noriyuki Nakamura and Kotaro Hirasawa.

ROUFF, Marc (Laboratoire de Génie Electrique de Paris, ESE, France)

The analytical computation of C^k spline spectra

C^k spline functions, i.e. spline functions which give as a finite sum a C^k approximation of desired functions, are presented in the framework of their algebraic and geometric properties. The resulting functional expansions of these C^k spline functions have, as main property, that the coefficients of these functional expansions are merely the all set of derivatives or of partial derivatives of the considered function up to the degree k at each point of discretization. The analytic computation of their Fourier spectra are presented and their first algebraic and geometric properties are presented.

VILJAMAA, Pauli (Tampere University of Technology, Finland)

Basis functions in soft computing

Different soft computing methods and some well-known approximation techniques are described in a unified framework, which makes it possible to point out the common areas and key aspects of the different approaches. The emphasis is put on the basis functions because they are the common element in all of these methods and they have a strong influence on the smoothness and on the computational requirements. Finite element method, neural networks, fuzzy logic, spline functions and wavelets are treated. Methods which the techniques utilize to obtain the parameters of the nonlinear mapping are reviewed. An example is presented where a distributed parameter system is solved by finite element method and, on the other hand, the solution of the system is approximated by perceptron, radial basis, and fuzzy networks. Comparisons of computing load and approximation accuracy are made between the methods. This is a joint work with Heikki N Koivo.

ALBOUSSIÈRE, Thierry (University of Cambridge, UK)

Stability and transition to turbulence of the Hartmann layer

A single parameter Re/Ha defines a Hartmann layer. Its linear and energetic stability has been analysed. The linear stability threshold is close to Lock's estimate ($Re/Ha \sim 5 \times 10^4$, *Proc. Roy. Soc.*, 1955) but the energetic stability threshold corresponds to $Re/Ha \sim 50$. Experimentally, a turbulent duct flow is laminarized when this ratio drops below 250 (Branover, *Magnetohydrodynamics*, 1967). This suggests that the stability of the Hartmann layer governs the behaviour of the whole flow and that large disturbances survive at much lower values of Re/Ha than the linear threshold.

This is a joint work with R J Lingwood.

BRANDENBURG, Axel (Department of Mathematics, University of Newcastle, UK)

Dynamo action in MHD turbulence

At sufficiently large magnetic Reynolds numbers turbulent hydromagnetic flows can exhibit self-induced dynamo action. There are many examples in astrophysics where this happens, and there is now enhanced activity in trying to establish dynamo action in laboratory experiments. Meanwhile, numerical simulations have contributed a great deal to understanding this phenomenon. In my talk I will discuss various simulations displaying dynamo action. Particular attention will be given to the generation of ordered, large scale magnetic fields. This phenomenon is related to the existence of an inverse cascade in hydromagnetic turbulence.

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BRANOVER, H (Ben Gurion University, Israel)

Similarities between MHD and atmospheric turbulence

The review of extensive experimental and theoretical studies of Magnetohydrodynamic turbulence and low magnetic Reynolds numbers reveals a number of peculiarities of such flows. Regarding integral characteristics the most important experimentally observed phenomena are leading to the conclusion that electromagnetic forces are causing a sharp decrease of eddy viscosity (up to the onset of negative eddy viscosity) and to the inversion of normal Kolmogoroff's energy cascade and strong changes in disposition of heat and mass. Measuring of local characteristics of MHD turbulence manifests enhancement of anisotropy, increase of turbulence intensity and generation of large structures. At earlier stages of the studies of above mentioned phenomena there was a suggestion to relate them to the tendency of turbulency to become two-dimensional (or quasi two-dimensional) in the plane perpendicular to the magnetic field. However if this would be true then typical for two-dimensional turbulence slopes (-3) should appear in the energy spectra and in reality this did not happen. Also direct local turbulence measurements indicated that the velocity fluctuations in the direction of the magnetic field do not vanish. Therefore a conclusion was made that the magnetic field leads to an enhancement of the initial helicity of turbulence. Theoretical studies also justify this assumption. Increase of helicity is leading to formation of large structures, drag reduction etc. It is also consistent with the peculiarities of energy spectra obtained experimentally.

All the above has a great degree of similarity with results obtained experimentally and theoretically regarding a number of geophysical phenomena, especially atmospheric turbulence. This gives a serious reason to suggests an analogy between MHD turbulence at low magnetic Reynolds numbers and atmospheric turbulence. This analogy certainly exists regarding features of the turbulent velocity field despite the fact that the physical nature of body-forces acting as MHD flows (electromagnetic forces) and in the atmospheric (Coriolis forces, density stratification) is different. A possibility exists to simulate large scale turbulent phenomena in the atmosphere using a small scale liquid metal MHD flow in the laboratory.

COWLEY, Martin D (Engineering Department, University of Cambridge, UK)

Suppression of buoyant motion melts

Suppression of buoyant motion is a desirable goal in a variety of situations where materials are being processed. Alboussiere et al. (1996 Phys. Fluids) high-lighted the importance of symmetry when a DC magnetic field is applied to damp buoyant motion. Without appropriate symmetry Hartmann layers may be "active", so that core velocities are of order Ha times the level with "inactive" layers. The present discussion will show that layers which are inactive with respect to the core may become active with respect to side layers. Wall jets of the type first discussed by Hunt (1965 J. Fluid Mech.) are formed.

CROSS, Mark (University of Greenwich, UK)

Free surface melting

Melting of pure and/or reactive materials at high temperatures can be achieved without a contact or at a significantly minimised contact area using the AC field magnetic confinement with partial or even complete levitation. The high energy consumption and the liquid shape stability problems are the well known difficulties for this technology. We describe a flexible numerical modelling technique for simulating the dynamics of the velocity and temperature fields by pseudo-spectral collocation method based on a continuous, non-orthogonal co-ordinate transformation. The dynamic stress boundary conditions at the free surface, the turbulent velocity field and the electromagnetic force volume distribution are particular features included. The method permits us to follow considerable changes in the free surface shape and the progress of the melting front. Application examples include a cylindrical crucible with free top surface, a cold crucible, the semi-levitation and levitation melting. This is a joint work with V Bojarevics, University of Greenwich.

DAVIDSON, Peter A (University of Cambridge, UK)

Low magnetic Reynolds number turbulence

Magnetic fields are commonly used in the metallurgical industries to suppress motion in casting and refining processes. The mechanism is straightforward. Motion across a magnetic field line induces a current and so mechanical energy is converted into heat via joule dissipation. However, the magnetic field not only suppresses large-scale eddies created by the turbulence, but also acts on the small scale eddies created by the turbulence. It is important, therefore, to be able to characterize the influence of a magnetic field on the structure of turbulence. Here we show that the conservation of angular momentum plays a crucial role, constraining the way in which the turbulent eddies may evolve. When the conservation of angular momentum is combined with an energy dissipation law, we obtain the MHD equivalent of Kolmogorov's energy decay law for freely decaying turbulence.

ERNST, Roland (EPM MADYLAM, CNRS, France)

Inductive metalothermic process for material manufacturing

Inductive cold crucible techniques now used at industrial scale for melting and casting of materials. A new process is presented which is a high temperature chemical reactor using an inductive cold crucible to produce pure materials (such as titanium) from their oxides. The inductive chemical reactor is composed of a mixture of molten salts, contained in a cold crucible with a liquid lithium layer floating on them. The reduction of metallic oxide powder produces solid particles which settle at the bottom inside another cold crucible where they melt and solidify into an ingot. numerical modelling and experimental results are presented. This is a joint work with Marcel Garnier.

ETAY, Jacqueline (EPM-MADYLAM, France)

Hot film anemometer measurements in a continuous caster mercury model

In slab continuous caster, two symmetrical jets are feeding a mould which exhibits a large aspect ratio L/e . Therefore, in the larger meridian plan of the mould, the molten metal flow presents four main vortices of characteristic velocity U . The interaction between the jets and this flow may lead to instabilities. DC magnetic field are used to control this instabilities and to brake the speed of the feeding jets. Using hot film anemometer technique, velocities are measured inside a 1/3 scale mercury model of a continuous slab caster. A DC field may be on or not. This field is maximum 3700 Gauss at the level of the free surface and decreases to 1000 Gauss near the point of the impact of the jets on the small side of the caster. It appears that the presence of the DC field does not affect the geometry of the vortices. But it reduces the instabilities. The spectrum of the kinetic energy is strongly modified as well as the STROUHAL number fL/U attached the upper vortices in the mold. Physical explanations are given. This is joint work with Cecile Guillaumin.

FAUTRELLE, Yves (INPG/MADYLAM, France and University of Waikato, New Zealand)

Stability of free surfaces submitted to an alternating magnetic field: A parametric resonance problem

We consider the stability of a horizontal liquid-metal free surface in the presence of a horizontal alternating magnetic field. A weak formulation is used to derive a generalised Mathieu-Hill equation for the evolution of surface perturbations. Previous studies which rely on time-averaging the electromagnetic force over one field cycle have predicted either a neutral behaviour or a generally weak instability. However, dropping that hypothesis leads to different conclusions. We find much larger growth rates near the resonances, where the surface wave frequency is an integral multiple of the field frequency. When the back reaction of the velocity field is taken onto account, we show that all waves are damped except those whose frequency is close to the field frequency. This is illustrated by some mercury experiments.

GILLON, Pascale (EPM-MADYLAM CNRS, France)

Processing of materials using intense magnetic field gradients

The development of superconducting magnets makes it possible to produce strong magnetic field gradients in an industrial setting. Two mechanisms can generate forces in a magnetic field gradient: the motion of an electroconducting medium which induces the Lorentz force and magnetization effect related to the magnetic susceptibility of materials in which originates the magnetic force. We will review different processes in which each or both of these forces are exploited such as levitation of massive metallic samples, inclusions separation from a flowing liquid metal or thermomagnetic convection phenomena.

MOREAU, Rene J (Lab. EPM-MADYLAM, CNRS and INP de Grenoble, France)

MHD quasi-2D turbulent shear flows under high magnetic fields

In the presence of insulating Hartmann walls, when the distance between them is small enough and the magnetic field large enough, any disturbance becomes 2D (except within the Hartmann layers) in a time which is very small by comparison with the eddy turn-over time. Then the dynamics of the turbulence is dominated by the singular properties of 2D turbulence, namely an energy transfer toward the large scales. The viscous and ohmic losses, only present within the thin Hartmann layers, are responsible for the main part of the damping. The results of an experiment performed with mercury in a magnetic field up to 6 Tesla are presented. The fluid flow, which is electrically driven, is essentially a shear between a rotating annulus and a central core at rest. The results demonstrate that a high level of turbulence is present, whatever high is the magnetic field, and exhibit the main characteristics of this unusual turbulence: thickening of the free shear layer, energy spectra with peaks (corresponding to the large coherent structures) and with an inertial range whose spectral law may be $k^{-5/3}$, k^{-3} or k^{-4} , depending on the importance of the magnetic field. Many other important properties, such as the Reynolds stresses and the transfer property of a scalar quantity such as heat have been measured with a fairly good accuracy.

MÜLLER, Ulrich (Forschungszentrum Karlsruhe, Germany)

Heat transfer enhancement by MHD-control

Generally magnetic fields are known to damp turbulent motions in an electrically conducting fluid and therefore it may be conjectured that heat transport is inhibited. But experimental investigations have shown that under certain conditions externally imposed magnetic fields may enhance heat transfer by promoting organised turbulent flow in the form of large scale quasi-two-dimensional vortices. Two experiments are presented where such an enhancement of heat transfer is demonstrated in forced flow and natural convection: In MHD rectangular duct flow, turbulence is created from the magnetic field by the increased shear in the sidelayer regions. The large-scale quasi-two-dimensional vortices confined in the turbulent side layers are effective in enhancing heat transport and therefore the temperatures at a heat loaded side wall are considerably reduced. When a horizontal magnetic field is applied to a thermal convection flow, three dimensional flow patterns are suppressed. The resulting pattern of quasi-two-dimensional convective rolls become less dissipative and the convective heat transfer is enhanced.

PERICLEOUS, Koulis (University of Greenwich, UK)

Computations and experiments in MHD turbulence

There is a lack of suitable turbulence models applicable to liquid metal magneto-hydrodynamic flows; yet, such flows are becoming common in metal processing applications. The strong anisotropy in velocity fluctuations caused by the magnetic field-lines makes the use of industry-standard two-equation models of the k-e family rather uncertain. In this study, we compare a zero-equation generalised mixing length model to variants of two-equation k-e model, as applied to the experimentally measured high Reynolds number liquid metal flow in a cylindrical container. The recirculating flow, typical to a variety of metallurgical applications, is generated by a moderate frequency AC coaxial coil. The flow boundaries are the solid container walls and a free top surface, where the usual wall functions are not directly applicable. The generalised mixing length model is shown to predict satisfactorily the experimental flow field with much less numerical effort and avoiding the problems of convergence and uncertain boundary conditions for the two-equation model.

THESS, Andre (Ilmenau University of Tech., Germany)

Numerical modelling of low RM turbulence

We report direct numerical simulations of the three-dimensional flow of an electrically conducting incompressible fluid under the influence of a homogeneous magnetic field at low magnetic Reynolds number. The behavior of the system is discussed for different values of the magnetic interaction parameter N . A novel intermittent regime is found for intermediate values of this parameter. This is joint work with O Zikanov, Dresden University of Technology.

WIDLUND, Ola (Faxén Laboratory, Royal Institute of Technology, Sweden)

MHD turbulence models for engineering applications

Magnetic fields have found wide-spread use in many industrial materials processing applications. In continuous casting of steel, for example, a static magnetic field is applied across the mould to control the melt flow. Numerical simulations of turbulent MHD applications suffer from the inability of conventional turbulence models to deal with the large anisotropies of length scales in MHD turbulence. The authors have proposed an extended Reynolds stress closure for modeling of turbulent MHD flows. In contrast to conventional Reynolds stress transport (RST) models, the new closure includes structural information which is vital for a correct description of MHD turbulence.

BRENIER, Yann (IUF and University Paris 6, France)

Homogeneous hydrostatic incompressible flows

The primitive equations used for the modelling of atmosphere and ocean dynamics are usually based on the hydrostatic assumption that the pressure field depends on the vertical coordinate in a rather trivial way. A rigorous justification of this popular assumption is not obvious from a mathematical point of view since it corresponds to a severe degeneracy (with respect to the horizontal coordinates) of the elliptic part of the equations. In the simple case of an inviscid incompressible motion in one horizontal space variable, we show that the hydrostatic equations are well-posed (for small time) provided that the initial horizontal velocity profiles are convex in the vertical variable. Of course, this condition is related to the classical Rayleigh stability criterion. It is also shown that the convexity generally breaks down in a finite time.

CONSTANTIN, Peter (The University of Chicago, USA)

The Littlewood-Paley spectrum in two-dimensional turbulence

We will describe the Littlewood-Paley spectrum - a dyadic average of the usual spectrum. We will present a proof of an upper bound for the spectrum near the dissipative cut-off as well as some numerical results confirming the bounds. Joint work with Q. Nie and S. Tanveer.

JONES, Christopher K R T (Brown University, USA)

Challenges in assessing Lagrangian transport in ocean flows

Reasonable modelling, even under simplifying conditions, of ocean flows requires numerical modelling that poses a considerable challenge to the dynamicist interested in implementing geometric Lagrangian techniques. This talk will be based on joint work with Pratt (Woods Hole) and Miller (Stevens Institute of Technology) on a study of circulation around an island. The fluid transport, and resulting vorticity budgets, associated with the dead zone off the eastern coast of the island will be discussed. Particular focus will be put on the numerical issues associated with the different levels of computation: solving the PDE itself and then the (numerical) velocity field as an ODE.

NICOLAENKO, Basil N (Arizona State University, USA)

Predictable unbalanced dynamics and ageostrophic wave fronts for geophysical flows

The 3D rotating Boussinesq equations (the "primitive" equations of geophysical fluid flows) are analyzed in the asymptotic limit of strong stable stratification. We describe classes of nonlinear anisotropic ageostrophic baroclinic waves which are generated by the strong nonlinear interactions between the quasi-geostrophic modes and inertio-gravity waves. In the asymptotic regime of strong stratification and weak rotation we show how switching on weak rotation triggers frontogenesis. The mechanism of the front formation is contraction in horizontal dimension balanced by vertical shearing through coupling of large horizontal and small vertical scales by weak rotation. Vertical slanting of these fronts is proportional to $\sqrt{\eta}$ where η is the ratio of Coriolis and Brunt-Väisälä parameters. These fronts select slow baroclinic waves through nonlinear adjustment of horizontal scale to vertical scale by weak rotation, and are the envelope of inertio-gravity waves. Mathematically, this is generated by asymptotic hyperbolic systems describing the strong nonlinear interactions between waves and potential vorticity dynamics. This frontogenesis yields vertical "glueing" of pancake dynamics, in contrast to the independent dynamics of horizontal layers in strongly stratified turbulence without rotation.

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ROULSTONE, Ian (Meteorological Office, UK)

Monge-Ampère equations in balanced models

We study 2-forms on phase spaces of hamiltonian models of nearly geostrophic flows. A quaternionic structure is identified, and the complex part of a symplectic representation of this structure corresponds to an elliptic Monge-Ampère equation. We review some of the ellipticity conditions that arise in potential vorticity inversion problems, and discuss applications of balanced models in numerical weather prediction and data assimilation schemes.

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GÜNTHER, Michael (TU Darmstadt, Fachbereich Mathematik, Germany)

PDAE models for electrical network simulation

In electrical network simulation, both real circuit elements and real interconnections are usually described by composing ideal, compact (i.e. non-distributed) circuit primitives, which have well defined terminal characteristics described by electrical parameter values. Examples are companion network models for transistors, which approximate the physical behaviour of semiconductor devices, or transmission line models, composed of RLC elements and controlled sources. This companion model approach corresponds to a spatial discretization of the underlying partial-differential equations (PDEs), and enables the inclusion of parasitic effects in a network model governed by differential-algebraic equations (DAEs). In my talk I will discuss an alternative approach: for elements as transmission lines and semiconductor devices refined network elements are allowed with PDE models as constitutive relations. Hence numerical methods can be tailored to the resulting model - spatial discretization is not already made at the modeling level. Mathematically, this ansatz yields coupled systems of PDEs and DAEs, or PDAEs, linking the PDE boundary conditions with the DAEs at the boundary nodes. The analysis and numerical treatment of such systems is an object of current research. Here one is especially interested in generalizing the DAE index concept to PDAE systems: first, to get a measure for the sensitivity of the system w.r.t. slight perturbations in initial values and input signals; and secondly, to estimate the resulting problems for numerical simulation. The talk will give an overview on the PDAE approach for network simulation by inspecting some instructive examples and introduce different PDAE index concepts. We will investigate whether some hints can be given on the impact of semidiscretization on index and properties of the approximative DAE systems.

HIGUERAS, Inmaculada (Universidad Pública de Navarra, Pamplona, Spain)

Numerical methods preserving contractivity

Given an ODE, it is well known that the methods that maintain the qualitative behavior of the solutions usually give better numerical results. The study of such methods for different classes of problems give rise to the different concepts of stability (*A*-stability, *B*-stability,...). A similar study can be done for DAEs. In this talk, we will give numerical methods that preserve contractivity for a class of DAEs arising in circuit simulation.

LAMOUR, René (Humboldt-University of Berlin, Germany)

Calculation of consistent initial values of lower index DAEs

The simulation of electronic circuits, chemical reactions or mechanical motions results in differential-algebraic equations (DAE) of different index. The numerical treatment of such equations needs the computation of consistent initial values. Using the splitting techniques suggested by the tractability index a system of nonlinear equations with nonsingular Jacobian is presented, which solutions are the consistent initial values for DAEs up to index-2. Examples show the applicability of the method.

SCHEIN, Oliver (Technische Universität Darmstadt, Germany)

Stochastic differential algebraic equations for noise in circuits

A physical model for thermal noise in resistors based on stochastic differential equations is included in circuit analysis with classical MNA. We analyze the structure of the resulting stochastic differential algebraic equations (SDAEs) and derive existence, uniqueness and limit theorems for all relevant indices. Numerical solution approaches are discussed. The results obtained reflect and clarify the well-known Nyquist rule for thermal noise in circuits from a mathematical point of view.

TISCHENDORF, Caren (Lunds University, Sweden)

Asymptotic properties of DAEs in circuit simulation

The asymptotic behaviour of solutions of DAEs is determined by the flow restricted to certain constraints. Integration methods like the BDF method and the Runge-Kutta methods can produce numerical solutions with an entirely other asymptotic behaviour as expected from the ODE point of view. If the constraints and the corresponding subspaces, respectively, vary with respect to the time then integration methods have problems to reproduce these variations correctly. This implies additional problems for the stepsize control of iteration methods. Here, we investigate the special class of DAEs which arises from the modified nodal analysis (MNA) in circuit simulation. We derive simple characterizations of the relevant subspaces. This allows us to present modelling criteria which guarantee that the numerical solution reflects the same asymptotical behaviour as the exact solution if we use the BDF method or a stiffly accurate implicit Runge-Kutta method.

ARRIDGE, Simon R (Dept. Computer Science, University College London, UK)

Topics in optical tomography

Optical Tomography is a method of imaging optical absorption and scattering coefficients inside living tissue. Several data acquisition schemes and reconstruction schemes have been proposed. In this talk we will concentrate on time-resolved measurement systems, and efficient computational schemes for the inverse problem based on Finite Element methods. In particular we consider: - the influence of different temporal and spatial sampling methods, - the influence of different reconstruction bases, - direct versus adjoint methods, - 2D versus 3D methods.

Examples from modelled and experimental data will be given.

DOBSON, David C (Texas A&M University, USA)

Determining periodic structures with maximal band gaps

Consider the problem of determining material arrangements in composite periodic dielectric structures, which result in maximal band gaps in the frequency spectrum for electromagnetic wave propagation. The approach proposed is to first formulate an appropriate optimization problem, which turns out to have a nonsmooth but Lipschitz continuous objective. A generalized gradient is then calculated, and a generalized gradient descent algorithm is proposed. Computational experiments are presented in which several new structures with large band gaps are obtained.

LESSELIER, Dominique (Laboratoire des Signaux et Systèmes, CNRS-SUPELEC-UPS, France)

On some computational issues in nonlinearized wavefield inversion

The paper will focus on nonlinearized wavefield inversion techniques tailored for the shape reconstruction or the mapping of unknown or partially unknown, penetrable and impenetrable objects in a planar-stratified embedding. Most of the attention will be devoted to so-called modified gradient techniques and specialized versions thereof, and to complete family methods, which all amount to the simultaneous minimization of the residuals of a data equation and of a state equation, with enforcing adequate constraints from a priori information. Emphasis will be on computational issues that arise when trying to apply them to the buried object configuration where aspect-limited data are the only ones available. This is a joint work with M Lambert.

SILTANEN, Samuli (Helsinki University of Technology, Finland)

Non-iterative impedance imaging: Applying Nachman's method

In 1996, A Nachman published a constructive solution to the 2D inverse conductivity problem. As this problem has important applications such as the medical imaging method called electric impedance tomography (EIT), it is interesting to design a numerical reconstruction algorithm based on Nachman's result. The talk describes the current status of such a project being carried out in collaboration with David Isaacson and Jennifer Mueller from RPI.

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BOISGÉRAULT, Sébastien (Ecole des Mines de Paris, France)

Shape sensitivity analysis for the Navier-Stokes equations

Regularity results with respect to the shape are derived for the pressure and the velocity fields that are solutions of the stationary Navier-Stokes equations: provided that the data are smooth enough and that the Navier-Stokes problem is non-singular in the initial domain, we obtain sensitivity results in the full spatial regularity. This allows us to perform the explicit calculation of the shape gradients of a class of functionals widely used by engineers, including both distributed and boundary functionals. This is a joint work with Jean-Paul Zolésio.

BUCUR, Dorin (CNRS, France)

Concentration-compactness principle and shape optimization

Given a sequence of open sets $(A_n)_{n \in \mathbb{N}} \subseteq \mathbb{R}^N$ of uniformly bounded measure, we prove a theorem of concentration-compactness type in $\mathcal{L}(L^2(\mathbb{R}^N))$ for the resolvent operators $R_{A_n} : L^2(\mathbb{R}^N) \rightarrow H_0^1(A_n)$, $R_{A_n} = (-\Delta)^{-1}$. We use this result for the proof of the existence of minimizing domains for some cost functionals depending on the eigenvalues of the Dirichlet-Laplacian. Particularly, we deduce that all sequences $(u_n)_{n \in \mathbb{N}} \subseteq H^1(\mathbb{R}^N)$, such that $u_n \in H_0^1(A_n)$, have a uniform behavior in $L^2(\mathbb{R}^N)$.

CAGNOL, John (Ecole des Mines de Paris, France)

Shape optimization for the Maxwell equation

We investigate the sensitivity of the solutions to the Maxwell equation with respect to the shape of the domain. We explicit a derivative with respect to a deformation parameter. The comparison with the corresponding results for the wave equation will be made. Application to the shape optimization and optimal design of antennae is considered as well as other industrial applications.

This is a joint work with Jean-Paul Marmorat and Jean-Paul Zolésio.

DÉTEIX, Jean (Université de Montréal, Canada)

Maximal slope stability of soils by use of reinforcing material: A shape optimization formulation

Certain methods for evaluating the possibility of a landslide can naturally lend themselves to a shape formulation. Here we maximize the stability (a safety factor defined via the limiting equilibrium method) for a given geological site (a pit slope). To do this we use a limited quantity of a given material (a reinforcing material) and we seek an optimal shape and position for this material in the pit slope. This approach can easily be applied to several engineering problem: design of retaining wall, road conception, drainage chimney in dam, etc. In this presentation we will give a formulation for this shape problem using characteristic function, theoretical results and some numerical results.

DZIRI, Raja (Université de Tunis, France)

Shape sensitivity analysis for nonlinear heat convection

We prove the material derivative existence for the solution of the stationary nonlinear heat equation arising in natural or mixed convections. We establish a differentiability result for the same operator when the coefficients are assumed to be independent of the temperature (the linear case). In both case we characterize de material derivative. This is a joint work with Jean-Paul Zolésio.

EPPLER, Karsten (Universitat Chemnitz, Germany)

Sufficient optimality conditions and applications to some shape optimization problems

A class of shape optimization problems for linear 2D-elliptic equations is considered by a special approach for the description of the boundary variation. In this way, together with methods of potential theory, the optimal shape design problem is transformed to an optimal control problem governed by a highly nonlinear integral equation, where the controls describe the parameterization of the boundary. We are able to show the existence of Fréchet-derivatives of first and second order of the *objective* w. r. to the control if all data are regular enough. Based on this, necessary and sufficient optimality conditions are investigated. In order to obtain sufficient optimality conditions, we have to overcome the so-called "two-norm-discrepancy", known from optimal control of ODE and PDE. Finally these conditions are applied for a discussion of a class of shape problems introduced by Belov and Fuji.

GOMEZ, Nicolas (Ecole des Mines de Paris, France)

Asymptotic behavior for the shape differential equation

Existence results for the Shape Differential Equation are derived, with specific attention for shape control problems. The particular case of gradient methods is investigated, and results are derived for a large class of problems, provided some continuity and uniform boundedness properties of the shape-gradient. The technique is illustrated on non-newtonian fluid flows, in order to decrease a cost functional. The asymptotic convergence of the domains towards a stationary one is obtained, provided a stronger shape continuity of the gradient. This is a joint work with Jean-Paul Zolésio.

HÖMBERG, Dietmar (Weierstraß Institute for Applied Analysis and Stochastics, Germany)

State constraint optimal control of laser surface treatments

We present a model that is capable of describing the solid-solid phase transitions in steel. It consists of a system of ordinary differential equations for the volume fractions of the occurring phases coupled with a nonlinear energy balance equation to take care of the latent heats of the phase changes. This model is applied to simulate laser surface hardening, which plays an important role in the manufacturing of steel. The aim of this heat treatment is to produce a martensitic layer on some part of the workpiece surface. We formulate this problem in terms of an optimal control problem. To avoid surface melting, which would decrease the workpiece quality, pointwise state constraints for the temperature are included. We discuss existence and stability results and derive necessary optimality conditions. To demonstrate the validity of the model, we conclude with some numerical results of laser surface hardening applied to the steel 42 CrMo 4.

This is a joint work with Juergen Fuhrmann and Jan Sokolowski.

FELGENHAUER, Ursula (Technical University Cottbus, Institute of Mathematics, Germany)

First- and higher-order Ritz methods for constrained optimal control

In the paper nonlinear optimal control problems with boundary and mixed inner constraints are considered. Using duality results by R. Klötzler et al., an indirect Ritz type discretization approach is derived and analyzed for its convergence. Under stable optimality conditions together with the continuity of controls and certain structural assumption on active constraint switches, for a first order method the convergence rate $O(h)$ is obtained. In the case of sufficiently smooth control regimes and for appropriate piecewise polynomial test functions the convergence rate is of higher order. The results fit well into the known theory of FE methods for ODE.

MAURER, Helmut (Westfälische Wilhelms-Universität Münster, Institut für Numerische Mathematik, Germany)

Sensitivity analysis for state constrained optimal control problems

Parametric nonlinear optimal control problems subject to pure state inequality constraints are considered. Conditions are given under which the optimal solutions are Frechet-differentiable functions with respect to the parameter. Sensitivity differentials of optimal solutions and adjoint variables are obtained by solving an associated linear boundary value problem. The computed sensitivity differentials are used to design real-time approximations of perturbed solutions via Taylor expansion. Numerical examples are provided that illustrate different features arising from the order of the state constraint. Two technical applications are discussed in more detail: (1) optimal control of the Van-der-Pol oscillator, (2) a crane loading model to control the swing angle.

OBERLE, Hans Joachim (Universität Hamburg, Institut für Angewandte Mathematik, Germany)

Optimal feed rates for a fed-batch fermentation model with state constraints

In this paper a model for a fed-batch fermentation process is considered which describes the biosynthesis of penicillin. The model is formulated as an optimal control problem with the feed rate as control variable. Numerical solutions are presented obtained by a new direct method which takes into account the expected switching structure of the optimal solution. The results are compared with solutions obtained by a standard indirect method (multiple shooting). Further, state constraints with respect to the biomass- and the substrate-rate are considered. The corresponding necessary conditions via optimal control theory are derived and numerical solutions of this extended problem are presented.

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PICKENHAIN, Sabine (Technical University Cottbus, Germany)

Optimal control problems with first order PDEs and state constraints

In this paper a Maximum Principle is shown for multiple integral problems of optimal control with first order PDEs and state constraints. It can be proved, that the canonical variables are measures from C^* , if the optimal control is assumed to be piecewise continuous. The theory is applied to the problem of warping of cross-sections under torsional stress.

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GELDER, David (Pilkington, UK)

The high temperature limit on glass fibre drawing

Glass fibre drawing is operated between a (cold) breakage limit and a (hot) stability limit. The high temperature instability is essentially a kinematic phenomenon, but influenced both by surface tension and the details of the (very complex) cooling regime. Various mathematical treatments have been proposed. A linear perturbation analysis will be presented, and the results compared with operating experience of multi tip bushings for continuous filament formation.

NEFEDOV, Seva (Department of Mathematics, Eindhoven University of Technology, Netherlands)

The glass tank model

Glass is produced in an oven. It is a rather complicated process where raw material is heated by burners. The heating process and the structure of the oven are designed in such a way that the melt remains in the tank for a certain period of time. Several techniques are used to obtain a uniform density such as electrochemical boosting and bubbling. We shall give a method to simulate the flow and heat transfer in this highly nonuniform region. Therefore we use a method that is based on local refinement and finite volume techniques. The eventual method is employing the simple datastructures of (local) uniform grids only.

SIEDOW, Norbert (Institute for Industrial Mathematics (ITWM), Kaiserslautern, Germany)

Applications of radiative transfer in glass industry

The knowledge of the exact temperature in semitransparent materials like glass is very important to control the production process. Numerical simulations could help to reduce the production costs. The heat transfer in these materials includes not only conduction and convection but also radiation. Since the coupling between the energy equation and the equation of radiative transfer is highly nonlinear, it is of great importance to use efficient and accurate solution procedures to the radiation part. We will give an short overview about the most important numerical methods for radiative transfer and different applications regarding to their accuracy and practicability. This is a joint work with Matthias Brinkmann, Schott Glas, Mainz, Germany.

TUCK, Ernest O (University of Adelaide, Australia)

Slumping of molten glass

Slumping of molten glass is used in the manufacture of windscreens and moulds for plastic ophthalmic lenses. It is best modelled using a fully numerical method, and we have developed a finite-element code for this purpose. Where the product is thin, asymptotic methods can yield supplementary information. We consider such asymptotic analysis of the slumping of thin nearly-flat glass sheets through distances of up to a few sheet thicknesses. Comparison with finite-element solutions for sheets of finite thickness indicates the extent of applicability of the thin-sheet analysis to real situations. This is joint work with Y M Stokes.

BERNADOU, Michel (Pôle universitaire Léonard de Vinci and INRIA, France)

Some results on modelization and approximation of piezoelectric thin shells

In this presentation, we report some new results obtained in the numerical modelization of piezoelectric thin shells. We successively consider: - the 3d modelization by using a set of general curvilinear coordinates and we obtain an existence and uniqueness theorem; - the derivation of 2d modelization - by integration through the thickness: we obtain an extension to piezoelectric thin shells of the Koiter equations valid for purely mechanical shells; - by using asymptotic methods; here again, we extend to piezoelectric thin shells the results obtained by Ciarlet and coworkers on purely mechanical thin shells; - the approximation by finite element methods of the model obtained in step This section takes into account the use of numerical integration and gives a priori error estimates. - some numerical examples proving the efficiency of the above results. - some comments on possible extensions to dynamical modelization and the use of such results to consider active structural control.

This is a joint work with Christophe Haenel.

HANSEN, Scott (Iowa State University, USA)

Modeling and control of plates with localized piezoelectric patches

We first describe a consistent variational formulation of a piezoelectric patch. Several possibilities arise, depending upon the types of assumptions used in the plate modeling and treatment of the electrical components. However, in each case the electrical components are retained as independent state variables. This allows one to easily obtain the appropriate variational boundary conditions. We then consider some possible models for a patch that is mounted on a portion of the surface of a plate. Again the problem has a variational formulation and all boundary conditions and edge conditions are easily obtained. Well-posedness and some possible control strategies will be discussed.

HENROT, Antoine (Ecole des Mines and Institut Elie Cartan Nancy, France)

Optimization of the shape of the actuators in an internal control problem

In this talk, we are interested in the optimization of the location and the shape of the internal control zone for an optimal control problem. As a model, we can consider the following wave equation

$$\begin{cases} \partial_{tt}u(x,t) - \Delta u(x,t) + \chi_\omega v(x,t) & = f(x,t) & \text{dans } Q_T = \Omega \times (0, T), \\ u(x,t) & = 0 & \text{dans } \Gamma \times (0, T), \\ u(x,0) = \partial_t u(x,0) & = 0 & \text{dans } \Omega. \end{cases}$$

where Ω is a bounded domain in \mathbf{R}^d , $d = 1, 2$ or 3 , ω is a subset of Ω which is the control zone, χ_ω is the characteristic function of ω , and v is an optimal control to be found. We can look at the following energy to minimize: $F(\omega, v) = \int_{Q_T} |\nabla u|^2 + (\partial_t u)^2 + \chi_\omega v^2 dxdt$.

In this talk, we will focus on the stationary version of the above problem. We consider different kinds of constraint on the control zone ω : a constraint on the perimeter or a constraint on the volume. In the first case, we prove existence of a minimizer and we give some property of it. In the second case, we show that it is necessary to relax the problem, but we give simple conditions on the data which ensure that the relaxed minimum is indeed a classical one (i.e. a characteristic function). At last, we give some examples of optimal control zones.

RAOULT, Annie (IMAG, France)

Relaxation results and applications to nonlinear shell models with directors

We use a variational convergence method to study the consistency of various Cosserat hypotheses in shell theory with the nonlinear membrane model derived from three-dimensional elasticity. We prove that using an affine approximation is correct, but that constraining the director to stay of norm 1 as is frequently done is inadequate. For the purpose of identifying the limit behavior of the director, we introduce a generalization of quasiconvexity that is suitable for problems with two vectorial unknowns, one of which appears through its gradient (the surface deformation), the other one through its value (the director field). This is a joint work with Hervé Le Dret.

RUSSELL, David (Virginia Tech, USA)

Issues in the formation of plates and shells by means of attached and embedded actuators

We report recent progress in our study of the control of the geometric configuration of linear elastic solids, as well as specializations to plates and other lower dimensional continua. We describe recent connections between optimal formation theory of two dimensional elastic bodies and conformal mapping and indicate some conjectures regarding the extension of these results to the three dimensional context as minimal shear mappings. Some numerical methods will be indicated and computational results will be presented.

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MSP-152

BOURQUIN, Frédéric (Laboratoire des matériaux et des structures du génie civil, UMR113 LCPC/CNRS, France)

Rapid stabilization of plates: A numerical analysis

Komornik's feedback law ensuring a rapid stabilization of a controllable linear system is investigated from the view point of the numerical analysis, in the case of thin plates controlled along part of their boundary by means of an imposed displacement or rotation. A "semi-weak" formulation of the problem is proposed in view of the space discretization. It is proved that the Fourier-Galerkin approximation leads to the prescribed decay rate of some energy of the plate uniformly with respect to the number of modes and the initial conditions. The numerical approximation of the control is explained and various numerical simulations are presented. They highlight the need for an enhancement of the original feedback law if control spill-over must be worried about. Such an enhancement is proposed and investigated. Komornik's feedback law ensuring a rapid stabilization of a controllable linear system is investigated from the view point of the numerical analysis, in the case of thin plates controlled along part of their boundary by means of an imposed displacement or rotation. A "semi-weak" formulation of the problem is proposed in view of the space discretization. It is proved that the Fourier-Galerkin approximation leads to the prescribed decay rate of some energy of the plate uniformly with respect to the number of modes and the initial conditions. The numerical approximation of the control is explained and various numerical simulations are presented. They highlight the need for an enhancement of the original feedback law if control spill-over must be worried about. Such an enhancement is proposed and investigated.

BRADLEY, Mary E (University of Louisville, USA)

Bilinear optimal control of a Kirchhoff plate via velocity controller

We consider a Kirchhoff plate with interior control of the form $h(t)w_t$, which acts as a bilinear control multiplying control $(h(t))$ by the velocity of the plate. We seek an optimal control of the plate to a desired evolution, z with cost functional $J(h) = \frac{1}{2} \left(\int_Q (w - z)^2 dQ + \beta \int_0^T h^2(t) dt \right)$. Special care must be given to the adjoint problem, since the admissible class of controls is only $L^\infty(0, T)$ and is not differentiable. Existence of optimal controls and uniqueness of such a control for T sufficiently small. This is a joint work with Suzanne Lenhart and Jiongmin Yong.

DUBEAU, François (Université de Sherbrooke, Canada)

Impulsive ODE and numerical approximation of such equations

When trains of impulse controls are present on the right-hand side of a system of ODE's, the solution is no longer smooth and contains jumps which accumulate at several points in time interval. So the solution at best belongs to the space BV of functions with bounded variation.

A fixed mesh variational formulation is used to establish existence and uniqueness of the solution of ODE's with (infinitely many state-dependent) impulses on the right-hand side. The asymptotic convergence of the approximation is proved and its order obtained.

This is a joint work with Michel Delfour.

HORN, Mary Ann (Vanderbilt University, USA)

Boundary controllability for coupled elastic systems

Information on the questions of boundary controllability and stability of complex structures is becoming increasingly important. Numerous results for single equations now exist, giving a well-established base of techniques. However, when more complicated, coupled systems are considered, new technical difficulties arise. Already, it has been seen that geometry plays a critical role in boundary controllability. This becomes even more apparent in complex systems. This presentation explores some of the challenges and the solutions to establishing controllability results for coupled systems of equations.

LAGNESE, John E (Georgetown University, USA)

Domain decomposition in exact controllability

We consider a dynamic network of one-dimensional elements such as a network of vibrating strings of Timoshenko beams. Control is applied at some of the exterior nodes of the network. It is assumed that the resulting controlled network is exactly controllable. Given a desired final state, the control of minimum norm that steers the system to this state is characterized by an optimality system that is obtained, for example, by the Hilbert Uniqueness Method. This optimality system for the entire structure is highly coupled and too complex for computational purposes. The main purpose of the talk is to demonstrate how this optimality system may be iteratively decomposed into subsystems defined on individual elements. The subsystems, which may be solved in parallel, are themselves optimality systems associated with certain optimal exact controllability problems on the individual elements. The iterations will be shown to converge to the solution of the global optimality system.

LASIECKA, Irena (University of Virginia, USA)

Control and design of structural acoustic models with thermoelastic effects

We consider a structural acoustic control problem modeled by coupled PDE's involving wave equation and plate equation with an interface on the boundary of two regions. The plate equation is described by linear Kirchoff theory accounting for thermal effects. We will show that in the presence of passive nonlinear damping applied to some walls of the acoustic chamber, the overall system is uniformly stable: ie the total energy decays to zero at the uniform rate. The present result should be contrasted with other stability results available for structural acoustic models where the walls were assumed to exhibit structural damping (Kelvin Voight type), making the the plate model analytic. In contrast, our results dispense entirely with the need for structural damping of the wall. As a consequence, the model considered is purely hyperbolic. The key role is played by the analysis of thermal effects which provide some sort of the dissipation of the energy which is then propagated onto the entire structure.

MCMILLAN, Christine (Virginia Tech, USA)

Optimal control problems for shells

In this talk, we consider linear quadratic regulator problems (in the presence of disturbances) for several shell models. In particular, we investigate problems with both control function ("good" player) and deterministic disturbance ("bad" player) acting on the boundary or at a point in the interior of the spatial domain. The optimal control and worst disturbance are synthesized in terms of a solution to a nonstandard Riccati equation. Specific examples include the cylinder, the cone, and the sphere with various boundary conditions.

SCHMIDT, Georg (McGill University, Canada)

On the controllability of vibrating mechanical structures from one equilibrium location to another

The talk will begin with a survey of various problems of the nature described in the title. These involve structures which can have a finite number of degrees of freedom (such as pendula of various kinds) and are then described by systems of nonlinear ordinary differential equations, as well as problems having infinitely many degrees of freedom (such as beams attached to rigid bodies and masses attached to cables) which involve partial differential equations. One system of the latter type will be discussed in greater detail with a view to illustrating the mathematical issues which arise in this area.

VALENTE, Vanda (IAC-CNR, Rome, Italy)

Relaxed exact controllability of thin and membrane shells.

We study the boundary exact controllability of the medium frequency vibrations of a thin shell. Spectral properties are considered, according to the spectral analysis for Douglas-Nirenberg elliptic systems of mixed order, and the fundamental role of the membrane approximation is shown. The relaxed spectral exact controllability result relies on an uniqueness theorem which is proved under suitable hypotheses on the middle surface of the shell.

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BRANDSTÄTTER, Wilhelm (AVL List GmbH, Graz Austria)

CFD in the automotive industry-solving today's problems and meeting tomorrows demands

The talk addresses state-of-the art approaches in the area of automotive fluid flow and combustion simulations. It will be demonstrated that the application of Direct Numerical Simulation (DNS) is far beyond the scope of today's available computing power when applied to real life industrial problems. Although Large Eddy Simulation (LES) seems to be a very attractive alternative in a mid-term perspective, there will be some difficulties pointed out which have to be overcome before it can be used on a routine basis. Therefore the remainder of the talk will focus on Reynolds Averaged Navier Stokes (RANS) solutions in connection with Differential Reynolds Stress (RMS) Turbulence and Probability Density Function (PDF) combustion models. Application examples will cover direct injection gasoline and diesel engine combustion, fuel injection systems and external car aerodynamics. At the end of the talk some future developments considered necessary will be addressed.

JEHLE, Erich (DaimlerCrysler AG, Germany)

Verification of university and commercial software-packages for the evaluation of car-wake structures

The first step of computing the quasi-unsteady 3D-structures in the wake of the SLK Mercedes Benz, based on the software packages STAR CD and KAPPA 10.0, is the verification of the numerical results with experimental measurements. Both CFD-Codes solve the set of non-linear equations with Finite Volume Methods and offer a variety of solvers and turbulence models, which resolve the near wall flow structures. The commercial product STAR CD from Computational Dynamic is a robust software package capable of modeling fluid flow, heat transfer, mass transfer and chemical reactions in industrial applications. KAPPA stands for a research code mastering flows in the real incompressible Mach-number region and in the hypersonic flows regimes. It offers artificial dissipation and a hybrid scheme from Jameson, as well as high resolution flux splitting schemes. The numerical results of the external automotive-flow are the starting point for the analysis of the fluid-mechanic structures in the car wake. Eigenvalues and eigenfunctions of the flow kinematics will be calculated from the numerical computation of the flow field to define and interpret singular points. The talk will focus on the question, if the flow structures and wake flow derived from the quasi-unsteady flow analysis is able to capture the real flow behavior, or is it indispensable to solve the unsteady Reynolds-averaged Navier-Stokes equations and time average these results. This is a joint work with U Dohrmann, Institute for Fluid Mechanics, University of Karlsruhe, Germany.

KLIMETZEK, Franz R (DaimlerCrysler AG, Germany)

Quality estimation for CFD at Daimler-Benz research

The availability of commercial codes for CFD even for small companies have led to a broad distribution and use of CFD in the industry. Despite the wide range of application it has to be stated that CFD has still not reached a mature state to be integrated in the series development for all types of problems. The experience showed that the main problem of accuracy in CFD comes from insufficient modeling partly from inadequate physical modelling, but mostly from numerical modeling and additionally from the interaction of both. The influence of the numerical error is often higher than the influence by switching to higher order physical models. Different estimators, together with an adaptive strategy were integrated to the 'Daimler-Benz Quality Estimation System'. This system is a tool to investigate the quality of the numerical solution and to obtain a solution that allows reliable answers to the designer's questions. This is joint work with Annette Jooss.

SANATIAN, Riaz (Chief Engineer, Computational Dynamics Ltd, London)

Practical aspects of CFD applications solving nowadays problems in the industrial design process

Star CD, as one of the leading commercial multi-purpose thermofluids analysis codes, has proved in a variety of practical industrial problems, while incorporating mathematical models and solvers which cover a wide range of thermofluids phenomena. From the perspective of a company designing a multi-purpose software package, the talk will focus on state of the art developments and limitations of physical models (e.g. turbulence and combustions models) solving practical problems in the chemical and automotive industry. In a short survey of industrial CFD-solution processes, starting from the grid generation for complex geometries, adapting the solver, to post-processing of the results, the aspects of mathematical accuracy versus robustness and the verification strategy will be highlighted.

NIETHAMMER, Barbara (University of Bonn, Germany)

Dynamics of the LSW mean field theory of coarsening

In the classical LSW theory Coarsening of a dilute systems of particles is modelled by a nonlocal conservation law for the particle size distribution function. LSW predict that the asymptotic behavior is self similar and that a particular smooth profile is approached.

In this talk we discuss rigorous results on the long time behavior of solutions to several variants of the model. For systems in which particle size is uniformly bounded these results establish a sensitive dependence on the data and thus in general do not confirm the predictions of the classical theory.

PENROSE, Oliver (Heriot-Watt University, Edinburgh, UK)

Mathematical models of nucleation and coarsening in alloys: An overview

This talk will review the physical background of the Becker-Doering and Lifshitz-Slyozov-Wagner equations and the mathematical relation between them, and any recent results that are not being dealt with by other speakers. I propose also to outline the (very striking) new effects that appear when elastic interactions are taken into account.

WATTIS, Jonathan (Division of Theoretical Mechanics, University of Nottingham, UK)

Modelling nucleation and growth of clusters with coarse-graining techniques

We derive a generalised Becker-Doring model of nucleation and cluster-growth. For size-independent rate constants, the use of matched asymptotic expansions enables an approximate solution of this microscopic model to be found. Approximating the microscopic model by a coarse-graining reduction yields mesoscopic, and ultimately macroscopic models of nucleation and growth. The solution of these models will also be described. As an example, a system in which clusters of two differing morphologies grow from the same monomer will be addressed; and, in particular, the case in which the less thermodynamically stable morphology nucleates first will be discussed.

BÄNSCH, Eberhard (Zentrum für Technomathematik, University of Bremen, Germany)

Crystal growth - a demanding application for flow simulation and free boundary problems

Semi-conductor crystal growth processes like Floating Zone, Bridgman and Czochralsky techniques are governed by the flow of the melt, the energy transport and the dynamic of interfaces. In order to optimize the process it is virtual to understand the diverse physical mechanisms and their relative influence. Due to the in-transparency of the melt simulations play an important role to understand and predict the behavior of the system. The mathematical model includes the Navier-Stokes equations in time dependent domains and a heat equation together with a free Stefan boundary condition for the interface liquid/solid and a free capillary condition at the interface liquid/gas. Joint work with B. Höhn, University of Freiburg, Germany

BENNER, Peter (Zentrum für Technomathematik, Mathematik und Informatik, Universität Bremen, Germany)

NICONET, a European network for numerically reliable software in computer-aided control systems design

NICONET (Numerics In Control NETwork) is a European thematic network with the aim of formalizing and extending current collaboration in the development of robust numerical software for control systems analysis and synthesis. As system complexity and ill-posedness of control problems in practical situations are rapidly increasing, more emphasis has to be given to the quality of the basic layer of numerical subroutines. Activities in the past have resulted in the control library SLICOT (Subroutine Library In Control Theory). This library is further developed, extended, and intergrated into CACSD environments within NICONET. Moreover, SLICOT subroutines are tested using industrial problems.

BINDER, Andreas (MathConsult GmbH, Austria)

Technomathematics for small and medium-sized enterprises

MathConsult GmbH is a mathematical software company, acting as a technology transfer institution between the Industrial Mathematics Institute (University of Linz, Austria) and industry. The transfer of mathematical expertise from university to SMEs often has to deal with the following specialities: - Typically, the partner within the company is not a mathematician but an engineer; therefore, the stage of mathematical modelling may be more time-consuming. - Limited budgets often make it necessary to introduce strong simplifications on the process to obtain a commercially acceptable solution.

We present our experiences and some case studies of projects carried out for SMEs.

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BÖHM, Michael (Universität Bremen, Zentrum für Technomathematik, Germany)

Chemically driven corrosion in concrete

Concrete surfaces such as sewer-pipe walls undergo chemical transformations causing irreparable damage to the pipes. They are due to the impact of various chemically active compounds. We consider a particular case - the formation of gypsum induced by the reaction of calcium and sulfide compounds in the porous concrete matrix. Problems like this can be modelled as moving boundary problems for systems of partial differential equations. In principle, the models yield corrosion speeds and other relevant information on that particular corrosion process. For several relevant cases the corrosion speed implied by the model coincides with 'real speeds'. Numerous questions are still open.

BUNSE-GERSTNER, Angelika (Zentrum für Technomathematik, Fachbereich 3/ Mathematik und Informatik, Universität Bremen, Germany)

Numerical steady state analysis of electronic circuits driven by multi-tone signals

Characteristics of analogue circuits such as intermodulation distortion and transfer characteristics can often be received from the steady state behavior. We present a unified approach for the simulation of non-autonomous circuits with multitone excitation. The system of ordinary differential-algebraic equations whose solution model the steady state are here changed into partial differential equations. The steady state is then derived from its solutions restricted to a line. Numerically solving the partial differential equation we are able to handle strong nonlinearities and widely separated time scales. Previous methods can be derived as special cases of this approach.

This is joint work with H G Brachtendorf, A Bunse-Gerstner, R Laur and G Welsch.

EGELJA, Aleksandra (Institute for Applied Mathematics, Freiburg, Germany)

Design tools for compressible viscous flow through two stroke engines

The viscous compressible flow through a two stroke engine will be considered. The aim of this project is the development of a software package (3-D) which can be used to improve (to optimize) the exchange process between fresh and burnt gas before the chemical reaction starts. The idea is to change the geometry of the cylinder and to study its influence on the exchange process. The compressible Navier-Stokes equations are discretised by a finite volume scheme on unstructured grids. We use Riemann-solvers for the discretisation of the convective terms and the discretisation which satisfy a maximum principle for viscous terms.

LANG, Patrick (ITWM, Germany)

Model reduction and robust filter design for elastomechanical systems

A large class of elastomechanical problems can be described in terms of highdimensional systems of second order ordinary differential equations, where the physical system parameters are comprised in highdimensional stiffness, mass and damping matrices.

For the filter design of those systems and in order to perform online simulations, appropriate model reduction procedures have to be applied first. Since moreover many of the system parameters are only vaguely known in general, the filter design has to be robust against the corresponding uncertainties. Therefore, a H_∞ -filter approach is presented, that is robust against a certain class of parameter uncertainties. The corresponding coupled algebraic Riccati equations thereby are solved iteratively.

LINDNER, Ewald H (Institute of Analysis and Computational Mathematics, University Linz, Austria)

Mass saving on an injection moulding machine and following projects

Commercial FEM packages in case of shape optimization are based on the description of the grid, in general. In contrast to this fact the description of the component requires only some parameters if the component is represented by some simple geometric primitives. Most of these packages are based on either direct solvers for the linear subproblems or on basic iterative solvers. Hence these codes are quite limited in their ability to properly consider critical regions of the PDE treated, e.g. in linear elasticity. This is a crucial problem especially for direct solvers for 3D-problems. During the past years the finite element package FEPP for 2D- and 3D-problems has been developed at our department. This code unifies most recent iterative solvers of multigrid type for PDEs with automatic adaptive grid refinement. We are considering nonlinear mixed integer constrained optimization originating from optimal shape problems. We will present the application to a problem of saving mass of the frame of an injection moulding machine. Hereby the machine is modelled as either the 2D-cross section or as a simplified 3D-body. The solution of the direct problem is to calculate the von Mises stresses. The constraints consist of requirements on limiting the stress in certain points and geometrical limitations. This is a joint work with Gundolf Haase.

WEISS, Martin G (ITWM Kaiserslautern, Germany)

Regulation thermography and long-term ECGs: Mathematics for diagnosis aiding in medicine

We present two applications of black box modelling in medical diagnosis aiding: In regulation thermography, temperature measurements on the surface of the human body are used for the diagnosis of diseases. Long term ECGs can be used to assess the risk of sudden cardiac death and related diseases. In both cases a large amount of data has to be considered to classify the measurements, a severe problem even for skilled human experts. Based on large amounts of training data mathematical methods from system identification and pattern recognition, ranging from statistics, fuzzy logic, neural networks to dynamical systems theory, are employed for data reduction and diagnosis aiding.

FASANO, Antonio (Department of Mathematics "U.Dini", Univ. of Florence, Italy)

Flows in porous media with hydrophile granules

Babies' diapers are porous media with the inclusion of hydrophile granules which can absorb water up to about 60 times this volume. The injection of water in such a system gives rise to a very complicated free boundary problem. One free boundary is the wetting front, followed by a saturation front, also unknown. Depending on possible constraints on the injection boundary conditions there may be more free boundaries on the inflow surface. The presence of a flowing phase and of a trapped phase (water absorbed in the granules) makes the rheological coefficients depend on the history of the flow. The corresponding 1-D problem has been studied, but so far only some partial result has been obtained and the whole topic appears to be an interesting source of problems, also from the numerical point of view.

HULSHOF, Josephus (Mathematical Institute of the Leiden University, The Netherlands)

Mathematical analysis of dynamic capillary pressure

We consider a new model for groundwater flow. The model differs from previous models in that the saturation-pressure relation is extended with a dynamic term, namely the time derivative of the saturation. The resulting model equation is of nonlinear degenerate pseudo-parabolic type.

BOHE, Adriana B (Weierstrass Institute For Applied Analysis and Stochastics, Germany)

Supersensitive internal layers in boundary and initial value problems

We study a class of singularly perturbed boundary and initial value problems exhibiting the phenomenon of supersensitivity. The shock layer behavior is very sensitive to perturbations of the boundary and initial values and of the coefficients in the differential operator. Using nonstandard analysis and a geometrical approach to describe the jumps of the associated fast-slow systems we determine sufficient conditions for the internal layer solution to exhibit either an exponential or an algebraic sensitivity. We also derive an ϵ -shadow expansion of the perturbed boundary or initial conditions that lead to an internal layer solution.

DMITRIEV, Michael G (Russian Peoples Friendship University, Russia)

Contrast structures in singularly perturbed optimal control problems

Contrast structures (trajectories with inner and boundary layers) in simplest vector variational problem and others optimal control problems in classical form are studied. Necessary optimality conditions lead to singularly perturbed boundary value problems for which contrast structures were not investigated before. Applying Krotov's formalism in the sufficient optimality conditions theory to these solutions lead to the new results in the contrast structures theory for special cases of ordinary differential equations. For example: structures of spike type are connected with points of local maximum and structures with inner passages are connected with the points of global maximum of some auxiliary problem function.

KALACHEV, Leonid V (University of Montana, USA)

Asymptotics of a Spike-Type solution

The boundary function method is used for construction of a spike-type solution of an elliptic equation in a two-dimensional domain.

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NEFEDOV, Nikolai (Moscow University, Moscow, Russia)

Asymptotic method of differential inequalities for problems with contrast structures

We present recent results on the method of asymptotic differential inequalities for problems with internal layers. We extend this method from scalar equations to systems of nonlinear singularly perturbed PDE's. For systems of parabolic equations we prove the existence of steady state solutions with internal layers and investigate their stability in the sense of Ljapunov.

SZMOLYAN, Peter (Institut für Angewandte und Numerische Mathematik, TU-Wien, Austria)

Geometric singular perturbation analysis of problems with exchange of stability

We consider singular perturbation problems with selfintersecting branches of the reduced manifold. Away from points of selfintersection the existing geometric singular perturbation theory is applicable. We present a new method based on blow-up techniques to analyse such problems near points of selfintersection. After passing near such a point a formerly stable solution can a) be attracted to the new stable branch, b) follow the old - now unstable - branch, c) be repelled away. In problems depending on parameters canard-solutions can be observed in an exponentially small interval of parameter values.

VASILIEVA, Adelaida B (Faculty of Physics, Department of Mathematics, Moscow State University, Russia)

Contrast structures arising by change of stability

The singularly perturbed PDE of parabolic type in some strip region is investigated. The right-hand part is periodic with respect to t , has the multiplier which is equal to zero at some point of the x -interval and changes his sign in this point. Under some conditions the problem may have the periodic solution which changes his form from the step type contrast structure to the solution having boundary layers only. The existence of such solution is proved.

CALVERT, Bruce D (University of Auckland, New Zealand)

1-networks

In this talk we introduce 1-networks, which are formed from infinite networks, with a time-flow relationship for each branch. Traffic may be, for example, considered to flow out of the ends, these flows summing to zero over equivalence classes of ends. Some basic theory is given.

GWINNER, Joachim (University of the Federal Army Munich, Germany)

Feasible flows in continuous transport and related constrained variational problems

In this contribution we study a continuum model of large dense discrete networks. Following the work of Taguchi and Iri, we embed the network in a (simply connected) bounded two-dimensional domain Ω . Then the unknown flow is described by a vector field, which has to satisfy the following constraints: the conservation law, capacity constraints like e.g. unilateral conditions in a subdomain of Ω and a nonlocal boundary condition to describe the given inflow rate of the source $S \subset \partial\Omega$. Here we make precise the functional analytical setting that permits to prove several new results.

As the first step of our extension of the classical Ford and Fulkerson network theory we treat the feasibility problem, that is, the characterization of the data that admit a feasible flow. In the next step we consider related constrained variational problems. The optimality conditions yield mixed variational inequalities which also lay down the basis for numerical discretization by mixed finite element methods.

MAUGERI, Antonino (Dipartimento di Matematica, Università di Catania, Italy)

Lagrangian function and duality for continuous models of traffic equilibrium

We are concerned with the traffic equilibrium problem in the continuous case, which is expressed by the Variational Inequality described Pr.(1): "Find $u^0 \in \overline{K}^{L^2(\Omega)}$ such that $\int_{\Omega} (Au^0 | u - u^0) + (B | u - u^0) dx \geq 0 \quad \forall u \in \overline{K}^{L^2(\Omega)}$ ", where $\overline{K}^{L^2(\Omega)}$ is the closure in $L^2(\Omega)$ of the set $K = \{u(x) = (u_1(x), u_2(x)) \in H^1(\overline{\Omega}, \mathbb{R}^2) \mid u_1(x), u_2(x) \geq 0, u_1(x)|_{\partial\Omega} = \varphi_1(x), u_2(x)|_{\partial\Omega} = \varphi_2(x), \operatorname{div} u + t(x) = 0\}$, the 2×2 matrix A and the 2-dimensional vector B define the cost functional $F(u) = \int_{\Omega} (A(u) + \frac{B}{2}(u)) dx$ and $t(x)$ is the density of the flow originating or terminating at x .

To this problem for which a lot of results are known, we apply recent techniques which allow us to obtain the Dual formulation of Pr. (1) and to associate to the solution of Pr. (1) the Saddle point of a suitable Lagrangian function. These results can provide new qualitative and computational properties of the equilibrium solution.

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NOZAWA, Ryôhei (Department of Mathematics, School of Medicine, Sapporo Medical University, Japan)

A formulation of continuous network and Gale's feasibility theorem

Iri formulated a continuous analog of max-flow min-cut problems in connection with an approximation of dense networks. On the other hand, Strang also introduced a slightly different type of continuous versions of max-flow min-cut problems and suggested a proper function space to deal with the problems. The function space is also applicable to Iri's problems. In this talk, we review the rigorous formulation of continuous network of Iri and Strang type and investigate a necessary and sufficient condition which assures the existence of flow satisfying some given constraints. This will be regarded as a continuous analog of Gale's feasibility theorem. There are some measure theoretical approaches to formulate continuous networks and Gale's feasibility theorem on them. In contrast to such approaches, our formulation must be closely related with regularity of a Euclidean domain occupied by a continuous medium and boundedness of the constraints for flows. We will relax the boundedness of the constraints of flows.

CINQUE, Luigi (Dipartimento Di Scienze Dell'Informazione, Università "La Sapienza" Roma, Italy)

Segmentation of page images having artifacts of photocopying and scanning

Without attention to the problems of print-through, marginal artifacts, and partial extra pages, the results of segmenting document images are poor. We have presented simple means for addressing each of these problems. We have demonstrated the effectiveness of our methods on a large database of real document images. In all cases, the print-through and marginal-artifact elimination techniques worked successfully. In 124 of 125 cases, the partial-extra page processing technique also worked well. Our methods are efficient in terms of computation time and space, an important consideration when processing high-resolution document images. Our methods should be practical for applications such as digital library development.



COSSU, Rossella (Istituto per le Applicazioni del Calcolo-CNR, Roma, Italy)

Document analysis experience in ancient books

Document image analysis applied to ancient documents can offer an important contribute for preserving and studying paper documents and book material. Page segmentation is used for the partitioning of the page into blocks constituted by groups of pixels having meaningful properties. A procedure of page segmentation using texture analysis for separating the blocks into text and no-text is presented. In a textured image the regions are described by repetition of different patterns. Local subpatterns repeated either deterministically or randomly can produce a texture viewed as a global pattern. The structure resulting from this repetition is used to discriminate various regions.

IMPEDOVO, Sebastiano (Consorzio Interuniversitario Nazionale per l'Informatica (CINI), Università di Bari, Italy)

Document analysis systems: State of the art and future trends

Documents analysis and handwriting recognition attracted the attention of researchers since the origin of computer. Nowadays, the technological progress made in the field of computer architectures and peripheral devices, as well as the advances of scientific research, make possible the development of new systems for document analysis and handwriting recognition. The lecture will present the State of the Art in this field and the new trends of the industrial and academic scientific communities. The most important algorithms for character, numeral and cursive word recognition will be discussed. Some of the most relevant future trends like the use of contextual processing, the multi-expert approaches and the CASE tools for systems design and development will be highlighted too.

LEVI ALDI, Stefano (Dipartimento Di Scienze Dell'Informazione, Università "La Sapienza" Roma, Italy)

Visualizing documents and their features

In many databases it is often difficult to know exactly which are its contents. One recent approach, borrowing from a previous project, displays the documents as points, forming clouds around well defined features (called points of interest or POIs). Some properties of documents (like number of authors, size in pages, pictures, etc) or contents (like key words) or structure (like sections, references) may be POIs. Using a given metric, points on the display near a POI represent documents having the POI feature. A view of the contents and structure of documents, as described in terms of their features, is obtained.

LOMBARDI, Luca (Dipartimento Di Informatica e Sistemistica, Universita' Pavia, Italy)

Segmenting documents by a multiresolution approach

In this work we propose a new page segmentation method for recognizing text and graphics based on a multiresolution representation of the page image. Our approach is based on the analysis of a set of feature maps available at different resolution levels. The final output is a description of the physical structure of a page. A page image is broken down into several blocks which represent components of a page, such as text, line-drawings, and pictures. The result, which uses only a small amount of memory in addition to that for the image, may be the first step for a more detailed analysis such as optical character recognition.

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CHAN, Tony F (University of California, Los Angeles, Department of Mathematics, USA)

Reduced Mumford-Shah models for image segmentation

This talk discusses approximations of functionals for image recovery and segmentation. The Ambrosio-Tortorelli and Shah approximations for the Mumford-Shah functional and a total variation minimization variant yield a system formed by two equations in two unknowns, the reconstructed image u and an edge-function v . These are continuously differentiable approximations. We show that we can reduce this system to only one equation in one unknown u , while still being able to extract the edges, and improve the sharpness of the edge-function v , and therefore of u as well. We finally generalize our approximations and present experimental results.

This is a joint work with L Vese.

FINZI VITA, Stefano (Università di Roma La Sapienza, Rome, Italy)

A Cahn-Hilliard evolution for planar curves in shape modeling

The evolution of closed planar curves is considered in Computer Vision with application to shape recovery. The initial set of curves matches a rough description of the contours of objects extracted by an image, and the evolution should have both a smoothing and a denoising effect. A well-known approach uses the Allen-Cahn equation from the phase transition theory to generate a mean curvature flow, with the effect of shrinking the smoothed curves. Here we propose, discussing its theoretical and numerical validation, a new level set approach to an area preserving geometric flow without shrinkage, based on the nonlinear Cahn-Hilliard model for phase separation.

MARCH, Riccardo (Istituto per le Applicazioni del Calcolo-CNR, Roma, Italy)

Visible surface reconstruction by using a second order variational method with free discontinuities

We consider a variational method proposed by Blake and Zisserman for image reconstruction. The method requires the minimization of a second order functional which depends on free discontinuities, free gradient discontinuities and second derivatives. We show how it is possible to approximate the functional by means of elliptic functionals in the sense of the De Giorgi Γ -convergence. An algorithm based on the elliptic approximation is applied to the problem of the reconstruction of visible surfaces from stereo images, and computer experiments on simulated images are presented.

This is a joint work with L Ambrosio and L Faina.

ROSATI, Mario (Istituto per le Applicazioni del Calcolo-CNR, Roma, Italy)

Convex-concave functionals in computer vision

In problems of computer vision two requirements may come into play whose compliance give rise to conflicting strategies. A typical example concerning the ratio of the colour intensity to the pixels distance is the need of smoothing jumps due to disturbances and enhancing jumps due to true contours. A possible strategy is given by minimization methods based on models with convex-concave regularizing functions. An important class of such models has been suggested by Geman and Mc Clure. Their asymptotical properties when the pixels number tends to infinity are presented in this lecture.

SPITALERI, Rosa Maria (Istituto per le Applicazioni del Calcolo, Rome, Italy)

Multigrid finite difference solution of Euler equations for variational image segmentation

We present a multigrid finite-difference approximation method to solve Euler equations for variational image segmentation problems. They are defined by the following basic steps: a-definition of the minimization problem of the Mumford-Shah functional (MSf); b-definition of the sequence of functionals Γ -convergent to MSf, c-definition and multigrid solution of the Euler equations associated to k-th functional of the sequence. We present results on method application to the solution of geometrical and real problems, along with evaluation of multigrid acceleration. This is a joint work with R. March and D. Arena.

VITULANO, Domenico (Istituto per le Applicazioni del Calcolo-CNR, Roma, Italy)

Numerical analysis of a nonconvex variational problem in image selective smoothing

We study some numerical properties of a nonconvex variational problem which is obtained as the continuous limit of a discrete method commonly used for image selective smoothing. The functional fails to attain a minimum value. Instead minimizing sequences develop gradient oscillations which allow them to reduce the value of the functional. The pattern of the gradient oscillations exhibits analogies with microstructures and it is analyzed numerically by using discrete parametrized measures. Some computer examples are also discussed.

This is a joint work with M Chipot and R March.

BJØRSTAD, Petter (University of Bergen, Norway)

PARASOL, A parallel library for large sparse linear systems

With the increase in computer speed and capacity, industry can apply computer simulation not only for verification purposes, but increasingly as an integrated step in the design and development cycle. Traditionally, industrial Finite Element codes have been quite problem specific and their algorithms for solving the linear equations have been tightly coupled to the rest of the code. The use of state of art algorithms is increasingly more important with growing problem size and more complex computer architecture, but the traditional 'in house' codes typically cannot afford the cost of frequent updates or even keeping up with the advances in (parallel) algorithms. The PARASOL project, funded by The European Commission, has attempted to address a part of this problem by the development of a library of algorithms for large sparse linear systems of equations. The library contains state of art methods, direct as well as iterative, and all algorithms should perform well on parallel computing platforms. The talk will describe overall library design, including the common interface to application codes. We will report on preliminary results from realistic industry generated test cases.

D'AMBRA, Pasqua (Center for Research on Parallel Computing and Supercomputers (CPS-CNR), Italy)

When PINEAPL met KIVA: Library usage in industrial applications

Numerical simulations of reactive flows are among the most computational demanding applications in the scientific computing world; the relevant codes are often difficult to maintain and improve, and the solution methods employed are also not always the most up-to-date. In this talk we focus on an activity carried out in the context of the PINEAPL project, funded by the European Commission. We have integrated some routines from the sparse solvers of the PINEAPL library in the KIVA-3 code, for simulation of chemically reactive flows in engine applications, obtaining some of interesting results, in terms of speed, efficiency, robustness and scalability. This is a joint work with Salvatore Filippone, IBM, Italy.

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DERAKHSHAN, Mishi (NAG Ltd, UK)

The PINEAPL project and the solution of sparse linear equations

The Numerical Algorithms Group Ltd is currently participating in the European HPCN Fourth Framework project on Parallel Industrial NumERical Applications and Portable Libraries (PINEAPL). One of the main goals of the project is to increase the suitability of the existing NAG Parallel Library for dealing with computationally intensive industrial applications by appropriately extending the range of library routines. Additionally, several industrial applications are being ported onto parallel computers within the PINEAPL project by replacing sequential code sections with calls to appropriate parallel library routines. A substantial part of the library material being developed is concerned with the solution of PDE problems using parallel sparse linear algebra modules. These modules provide support for crucial computational tasks such as graph partitioning, preconditioning and iterative solution of linear systems. Additional support routines assist users in distributing and assembling the data structures used and/or generated by the sparse linear algebra modules. This talk will provide a number of performance results which demonstrate the efficiency and scalability of core computational routines - in particular, the iterative solver, the preconditioner and the matrix-vector multiplication routines. Most of the software described in this paper will be incorporated into Release 3 of the NAG Parallel Library.

DUFF, Iain S (Rutherford Appleton Laboratory, UK)

Sparse matrix software in the Parasol project

PARASOL is an ESPRIT IV Long Term Research Project whose main goal is to build and test a portable Library for solving large sparse systems of equations on distributed memory systems. There are twelve partners in five countries, five of whom are code developers and five end users. The software is written in Fortran 90 and uses MPI for message passing. There are routines for both direct and iterative solution of symmetric and unsymmetric systems. The final Library will be in the public domain. We will discuss the PARASOL Project with particular emphasis on the algorithms and software for direct solution that are being developed by RAL and CERFACS. The underlying algorithm is a multifrontal one with a switch to ScaLAPACK processing later in the factorization (and solution). We will discuss the algorithms, the interface and their current status, and show their performance on some test problems provided by the end users. We will discuss some work on the effect of ordering schemes on load balancing and factorization performance.

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DICARLO, Antonio (Università degli Studi "Roma Tre", Italy)

How to model distensible blood vessels

This communication is based on joint work with Paola Nardinocchi and Luciano Teresi. We propose to model distensible blood vessels as one-dimensional continua, each point of which is a two-dimensional affine body, mobile in a three-dimensional Euclidean environment (or, to put it differently, as rods whose cross sections can stretch homogeneously in their plane). We claim that this one-dimensional theory - with properly tuned constitutive prescriptions - is supple enough to capture the essential features of blood-vessel mechanics, without overburdening the coupled model with the punctilios of three-dimensional elasticity, or of a two-dimensional shell theory. Therefore its implementation should prove helpful when computing solid-fluid interactions in blood flow. After presenting the basic ingredients of the theory, we concentrate on the strategy to use for coupling two structurally heterogeneous models: a standard 3-D continuum model for the fluid, say, *vs.* our 1-D continuum with affine microstructure for the vessel.

HILL, Nicholas A (Department of Applied Mathematics, University of Leeds, UK)

Modelling the interaction between blood flow and atherosclerosis

The thickening of the intimal layer of arteries which is a precursor to atherosclerosis is related (i) to transport of protein molecules across the endothelium which lines the artery and (ii) to the effects of low wall shear stress (WSS) on the permeability of the endothelium. In turn, the thickening changes the local geometry of the artery and affects the flow of blood and the WSS. We present results from a three-dimensional mathematical model which incorporates all of these effects and investigate under what conditions damage to the endothelium will lead to uncontrolled intimal thickening.

NOBILE, Fabio (Departement de Mathematiques, Ecole Polytechnique Federale de Lausanne, Switzerland)

Numerical modelling of fluid-structure interaction problems in hemodynamics

We address the numerical treatment of the the mechanical interaction between blood and vascular walls. The coupled fluid-structure problem is highly non linear and its well-posedness will be briefly discussed. We present some results obtained recently in the following fields: accuracy of Arbitrary Lagrangian Eulerian (ALE) formulations for Navier-Stokes equations; relationships between ALE approach and Space Time Finite Element Method for moving boundary problems; different strategies for coupling fluid and structure solvers. Numerical results will be presented about fluid-structure interaction simulations, based on simplified models for the mechanical behavior of the vascular tissue. This is a joint work with L Formaggia, EPFL.

PEDRIZZETTI, Gianni (Dept. Civil Engineering, University of Trieste, Italy)

Laminar separated flow in irregular ducts with elastic walls

Fluid flow in elastic conduits has a high theoretical and practical relevance but its calculation reserves many difficulties. The development of numerical techniques and the analysis of associated phenomena are the motivations of this work. The analysis is performed through the simultaneous numerical solution, in the axisymmetric approximation, of the incompressible Navier-Stokes and the full membrane equations (Pedrizzetti 1998, JFM 375); a simplified perturbative technique is also presented. The system stability and its unsteady resonance is analysed. The qualitative relevance of the inlet and outlet boundary conditions is also discussed.

PEIRÓ, Joaquim (Department of Aeronautics, Imperial College of Science, Technology and Medicine, UK)

Simulation of blood flow using high-order spectral elements on unstructured grids

In modelling the flow in the large arteries (with diameters of millimeters or above), it appears that the overall behaviour is most affected by the basic geometry and the unsteadiness of the flow. Arterial geometry is however complex, involving 3D curvature and frequent branching. The details of the velocity distribution are of considerable interest, particularly in relation to arterial physiology and disease. For some time a link has been postulated between low shear stress and the development of atheromatous lesions; more recent in vivo results reinforce the hypothesis of an association between related flow-derived parameters (long particle residence times, degree of shear reversal) and atheroma formation and development. It has also been found that the arterial walls respond directly to the shear stress exerted by the flow, through alignment of the cells lining the inner wall (or endothelium), and the production of vasoactive chemicals. Furthermore relatively stagnant flow regions are found to be more prone to thrombogenesis. This paper is concerned with the computational modelling of arterial flows using high-order numerical flow solution methods implemented on unstructured grids. The focus of the study is the haemodynamics of arterial bypass grafts and, in particular, the investigation of the effect of graft curvature in the shear distribution on the wall of the host artery.

PONTRELLI, Giuseppe (IAC-CNR, Italy)

A mathematical model for wave propagation in elastic tubes

Fluid motion in elastic tubes and its interaction with the wall is the basis for analyzing blood flow in arteries. Being interested in the propagation of pulses, the momentum equation is averaged over the cross-section, while the artery wall is modelled as a non-linear elastic membrane. The resulting system of P.D E.'s is solved by a second order finite difference method. Though quasi-1D, this wall law is not restricted to small deformations and is able to describe the fundamental phenomena. In particular, damped oscillations of the membrane, stability conditions and possible resonance effects are studied.

VENEZIANI, Alessandro (University of Verona, Italy)


Boundary issues for blood flow problems

In numerical hemodynamics, the boundary treatment of artificially truncated domains is a major issue. The flow equations demand for suitable pointwise conditions, mathematically admissible but seldom available. Measurements can provide integrated quantities on vessel sections, not enough to "close" the NavierStokes system. We investigate a mathematical setting for these defective boundary conditions. A more advanced approach, based on coupling the previous system with a lumped parameter model of the cardiovascular system, is addressed. Non-reflecting boundary conditions for the fluid-structure interaction problem, aiming at controlling the pressure waves originated by the compliance is considered. This is a joint work with Prof A Quarteroni, EPFL.

ZANETTI, Gianluigi (CRS4, Italy)

Viva: The virtual vascular project at CRS4

The aim of the ViVa project is to develop tools for the modern hemodynamicist and cardiovascular surgeon to study and interpret the constantly increasing amount of information being produced by non-invasive imaging equipment. In particular, we are developing a system that will be able to process and visualize 3D medical data, to reconstruct the geometry of arteries of specific patients and to simulate blood flow in them. The initial applications of the system will be for clinical research and training purposes. In a later stage we will explore the application of the system to surgical planning. ViVa is based on an integrated set of tools, each dedicated to a specific aspect of the data processing and simulation pipeline: image processing and segmentation; real-time 3D volume visualization; 3D geometry reconstruction; 3D mesh generation; blood flow simulation and visualization.

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CALINI, Annalisa (College of Charleston, USA)

Spectra, multi-phase solutions of vortex filament flow, and knot types

The Localised Induction Equation (LIE) describes the integrable self-induced dynamics of vortex filaments in an ideal fluid. We exploit the well-known connection between the solutions of the focusing Nonlinear Schroedinger equation and the LIE to explore the geometrical and topological properties of closed multiphase solutions. In particular we use methods of algebraic geometry, Backlund transformations and perturbation theory to construct first order perturbations of unstable elementary periodic solutions, whose Floquet spectra have real and complex double points. We discuss connections between different periodic perturbed solutions and the knot types for associated closed vortex filaments. This is a joint work with Thomas A Ivey, Ball State University, USA.

CRUZ-PACHECO, Gustavo (National Autonomous University of Mexico (UNAM), Mexico City, Mexico)

Approximate evolution of lump initial conditions for the Benjamin-Ono equation

In this talk we will study the approximate interaction between a soliton and the dispersive radiation in the Benjamin-Ono equation. This will be done by modulating a lump initial condition and using the conserved quantities to include the dispersive radiation. It will be shown that there is a very good agreement between these solutions and the full numerical solutions of the Benjamin-Ono equation, both in the temporal evolution of the soliton amplitude and in the final soliton stage for a wide range of initial conditions.

LEMESURIER, Brenton (College of Charleston, Charleston, USA)

Dissipation in singular blow-up solutions of the nonlinear Schrödinger equation

Energy transfer in plasma turbulence and from high-intensity laser beams due to multi-photon absorption can be modelled by a Dissipative perturbation of the Nonlinear Schrödinger Equation (DNSE). Numerical study of near-singular solutions of the DNSE in the limit of dissipation coefficient approaching zero suggest that sustained dissipative behaviour is possible in parameter regimes where it was not previously expected, related to singular solutions of the NSE, and reveal dissipation in a rapid train of bursts despite the steady form of the NSE limit. These solutions are related to special singular solutions of the NSE having dissipation into a point singularity.

OSBORNE, Alfred R (Dipartimento di Fisica Generale dell'Universita', Torino, Italy)

Theta functions and freak waves in the north sea

Recent ocean wave measurements made on an offshore platform in the North Sea have revealed the single largest surface wave ever systematically observed: 26 m from trough to crest. These surprising results have triggered a renewed interest in the occurrence of "rogue", "freak" or "giant" waves in the ocean. We develop a numerical approach for studying the hydrodynamics of extreme waves and use the inverse scattering transform for the nonlinear Schroedinger equation to analyze the data. This has required the development of computer codes for the entire Kotljarov-Its-Tracy formulation of IST, including solutions of the hyperelliptic flow and theta functions. We have been able to associate rogue wave activity with imaginary axis modes in IST and have found single and phase locked (breather) unstable wave trains in the data. Work on the prediction of rogue waves, using IST, is now underway.

SCHOBER, Constance M (Old Dominion University, USA)

Chaotic dynamics for symmetry breaking perturbations of the nonlinear Schrödinger equation and applications to water waves

Water waves on deep water are studied using the Nonlinear Schrodinger equation with higher order correction terms (HONLS). Numerical simulations of HONLS indicate that a novel type of chaotic dynamics develops which is qualitatively similar to results obtained in physical experiments. The inverse spectral theory of the NLS equation is used to interpret the numerical and experimental results.

ALEXANDRE, Radjesvarane (Universite d'orleans France)

Around Boltzmann equation without cutoff

We wish to present some recent (say two years) mathematical results dealing with Boltzmann models, when one does not assume Grad's cutoff hypothesis. As one knows (at least for the specialists) almost any earlier results do assume that hypothesis.

AOKI, Kazuo (Kyoto University, Japan)

Numerical analysis of a rarefied gas flow induced near the edges of a uniformly cooled or heated plate

A steady flow of a rarefied gas induced near the edges of a uniformly cooled or heated plate is analyzed numerically by an accurate finite-difference method on the basis of the Boltzmann-Krook-Welander equation. The behavior of the gas (the velocity and temperature fields, the propagation of discontinuities in the velocity distribution function, etc.) is clarified for a wide range of the Knudsen number (Kn). In particular, it is shown that for small Kn the flow is likely to be of $O(Kn^{1/2})$ and therefore has a larger effect than the thermal creep and nonlinear thermal stress flows of $O(Kn)$. This is a joint work with Yoshio Sone, Kentaro Ueda, and Shigeru Takata.

BANASIAK, Jacek (Department of Mathematics and Applied Mathematics, University of Natal, Durban, South Africa)

An interplay between elastic and inelastic scattering operators in models of extended kinetic theory and their hydrodynamic limits

We consider the space dependent linear Boltzmann equation for Lorentz gas with elastic and inelastic collision terms. Models of this type have been recently developed in semiconductor theory and extended kinetic theory. We analyze several versions of this equation corresponding to various collision operators being dominant (or acting on different time scales), and derive hydrodynamic limit for each version. It turns out that the type of hydrodynamic limit equation varies from case to case. We investigate properties of limit equations, show the convergence in each case, and provide numerical illustration of theoretical results.

FREZZOTTI, Aldo (Dipartimento di Matematica, Politecnico di Milano, Italy)

DSMC simulation of granular flows in planetary rings

The granular flow occurring in a planetary ring is studied in the framework of Enskog kinetic theory of dense fluids. Extending a previous investigation, the effects of the gravitational interaction among the granular particles is taken into account for a better comparison with existing studies based on molecular dynamics. The mathematical model is based on the Enskog kinetic equation which governs the evolution of the one-particle distribution function of an assembly of rough spherical particles undergoing anelastic collisions. The Enskog equation is solved by a DSMC-like particle scheme which includes the computation of the gravitational self-consistent field. Particular attention is devoted to the formation of particles clusters. This is a joint work with P Grosfils, CNLPCS, University of Bruxelles.

GROPPI, Maria (Department of Mathematics, University of Parma, Italy)

Chemical reactions and inelastic transitions in extended kinetic theory

A kinetic approach is presented for the analysis of a gas mixture with two kinds of non-conservative interactions. In a bimolecular chemical reaction mass transfer and energy of chemical link arise, and in inelastic mechanical encounters molecules get excited or de-excited due to their quantized structure. Molecules undergo transitions between energy levels also by absorption and emission of photons of the selfconsistent radiation field. From the kinetic Boltzmann-type equations, the problem of equilibria and of their stability is addressed. A detailed balance principle is proved and a Lyapunov functional is constructed; mass action law and Planck's law of radiation are recovered.

This is a joint work with Spiga Giampiero, University of Parma, Italy.

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LAMPIS, Maria (Dipartimento di Matematica, Politecnico di Milano, Italy)

A new model for the boundary conditions of the Boltzmann equation

In the literature some experimental data are available about the drag coefficient of monatomic gases at high energies (satellite experiments), or at low energies (laboratory experiments). In this paper a model for the velocity distribution function of the molecules reemitted by a solid wall, on which a monatomic gas is impinging, is proposed. According to this model the velocity distribution function is given by a linear combination of a shifted Maxwellian, containing two adjustable parameters, and of a Maxwellian in equilibrium with the wall. The model is applied to the calculation of the drag coefficient in free molecular flow. A comparison of the predictions of the theory with the data for the drag coefficient is made, obtaining satisfactory results. The abovementioned distribution function can be obtained by a very simple "scattering kernel".

SONE, Yoshio (Department of Aeronautics and Astronautics, Graduate School of Engineering, Kyoto University, Japan)

Bifurcation and stability in the cylindrical couette rarefied gas flow with evaporation and condensation

A rarefied gas between two coaxial circular cylinders are considered. The cylinders are made of the condensed phase of the gas, and the inner cylinder is rotating at a constant angular velocity. In our previous paper, we consider the problem under the assumption the behavior of the gas is circumferentially and axially uniform and present a new kind of bifurcation of flow under this simple situation. In the present paper, relaxing the assumption of the axial uniformity, we study the stability of the flows obtained under the assumption of axial and circumferential uniformity by the direct simulation Monte Carlo method, and clarify the type of stable solutions in the parameter space of the problem, including a new type. This is a joint work with Akihisa Okuda and Taku Ohwada.

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BEN AMAR, Martine (Laboratoire de Physique Statistique, Ecole Normale Supérieure, France)

Finger-fracture behaviour of a shear-thinning fluid in a Hele-Shaw cell

We present a theoretical treatment of the Saffman-Taylor instability when the displaced fluid is non-newtonian. For power-law viscosities, we face the problem of having a pressure field which is p-laplacian. By means of an hodographic transformation, we are able to handle the viscous-fingering instability in the limit of weak-shear thinning. Our results predict a finger width which decreases towards zero with the capillary number in agreement with various experiments.

CHAPMAN, S Jonathan (Mathematical Institute, Oxford University, England)

Capillary waves in zero gravity ploughing flows

The talk will describe the application of exponential asymptotics "beyond all orders" to the problem of a zero gravity ploughing flow with small surface tension. I will show that there are Stokes lines in the asymptotic approximation of the solution across which capillary waves of exponentially small amplitude are switched on. The position on the free surface at which these waves appear turns out to be governed by a strikingly simple rule.

The asymptotic results will be compared with the numerical results of J.M. Vandenbroeck.

COOKER, Mark J (University of East Anglia, UK)

Some theoretical and computational work on violent jet flows

This work was motivated by the impact of sea waves against coastal structures and the plumes of spray which impacts make. Two-dimensional unsteady free surface motion has been computed with a high-order time stepping method. The flow is ideal and free of surface tension but includes gravity. This boundary-integral method has produced results including a thin, high-speed jet erupting from the waterline, whose initial acceleration, can be 10,000g. This work attempts to relate the speed and width of the emerging jet from the pressure field which is associated with the fluid acceleration.

HOWISON, Sam (OCIAM, Mathematical Institute, Oxford University, UK)

Stokes flow with free surfaces

Stokes flow in two dimensions can be treated using complex variable techniques. I shall discuss some explicit solutions to free surface problems, with and without surface tension. I shall also discuss the connection between this problem and the Hele-Shaw problem.

This is a joint work with L M Cummings and J R King.

KING, Andrew C (School of Mathematics and Statistics, University of Birmingham, UK)

The formation and motion of a three phase contact line in a viscous fluid

We consider the formation of an unsteady three phase contact line when a thin, flat plate meets a planar gas/liquid interface. We include the effect of viscosity and use the theory recently proposed by Shikhmurzaev (in *Moving contact lines in liquid/liquid/solid systems*, J. Fluid Mech., 334, 211-249, (1997)) to modify the no slip boundary condition in the neighbourhood of the moving contact line. Singular perturbation methods are used to solve this problem in the limit of small capillary number. In particular we determine the contact angle as a function of the contact line speed explicitly. This is joint work with John Billingham.

TUCK, Ernest O (The University of Adelaide, Australia)

A generalisation of the Benjamin-Ono equation

Long waves $y = h\eta(x)$ of speed c on the interface $y = 0$ between a thin lower layer of heavy fluid (density ρ_1) and a light upper fluid (density $\rho_2 \ll \rho_1$) extending to $y = +\infty$ satisfy

$$-2 \left[\frac{c}{c_0} - 1 \right] \eta(x) + \frac{3}{2} \left[\eta(x) \right]^2 + \frac{1}{3} h^2 \eta''(x) + \frac{\rho_2}{\rho_1} h \mathcal{H} \eta'(x) = \frac{3}{2} \eta^2,$$

where \mathcal{H} is a Hilbert transform. Comparison is made between numerical results from the above equation and exact periodic wave computations, and also with analytic results of the Korteweg-de Vries and Benjamin-Ono equations, which are special cases. This is a joint work with L Wiryanto.

VANDEN-BROECK, Jean-Marc (University of East Anglia, School of Mathematics, UK)

Ripples on gravity-capillary free surface flows

Many free surface flows are characterised by the presence of small ripples in the far field. These include gravity capillary solitary waves, flows under a sluice gate and long bubbles rising in a fluid. The ripples can be of constant or decaying amplitude. We present examples of flows where the amplitude of the ripples is related to singularities in the intersection of free surfaces with rigid walls.

AZAIÉZ, Mejdí (Université Paul Sabatier, IMFT, France)

New Goda projection algorithm for the spectral element discretization of the Stokes equations

The subject is to present a family of projection methods applied to unsteady Stokes problem. They are intermediary between the Uzawa algorithm and the classical Goda time scheme and requires two steps. In the prediction-diffusion part a velocity and an intermediary pressure are computed by the uniformly div-stable bernardi-Maday spectral element (with few degrees of freedom on the pressure). the correction-projection step is made in the usual way to obtain the final velocity and pressure fields, also by spectral discretization. The first sub-problem is solved using the non-conforming decomposition mortar method while the second is inverted only locally rendering this step completely parallelizable. A numerical discussion will be carried out based on some computational experiments, proving the reliability of such approach.

BEN BELGACEM, Faker (MIP, Université Paul Sabatier, Toulouse, France)

Inf-sup conditions for the mortar spectral element discretization of the Stokes problem

The subject is to extend the inf-sup condition to the general case of nonconforming decompositions, with the help of the Boland and Nicolaides argument. We consider two situations: • a fixed decomposition, • a hierachical family of decompositions.

Even if this is not completely general, it includes a number of applications of the mortar method, for instance complex geometries where the decomposition is enforced by the aspect ratio of the domain and mesh adaptativity. In each case we first prove a basic result on the global domain. Next we use it to establish the uniform inf-sup condition i.e. the best possible constant in the inf-sup inequality only depends on the local inf-sup constants on each subdomain. We apply this condition to prove that the discrete Stokes problem is well-posed, then to derive optimal error estimates between the exact and discrete solutions.

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BERNARDI, Christine (Analyse Numérique, CNRS & Université Pierre et Marie Curie, Paris, France)

The mortar method in nonstandard Sobolev spaces

We present two applications of the mortar spectral element method to problems for which the variational spaces are no longer standard Sobolev spaces but the domains of either of the curl or divergence operators: the resolution of the Darcy's system for porous media and the computation of the vector potential. Our aim is to present the new arguments that are needed for the analysis of the mortar technique in this framework together with some numerical experiments.

BERTOLUZZA, Silvia (Istituto di Analisi Numerica del CNR, Pavia, Italy)

Substructuring techniques for mortar wavelets methods

In the framework of the Mortar Wavelet Method we will consider Preconditioning by *Substructuring*. The unknowns will be divided in *interior*, *edge* and *vertex*, and different block diagonal preconditioners will be tested for which the following asymptotical estimate can be proven: $\text{cond}(P^{-1}A) \leq C(1 + \log(H/h))^4$. Different choices of the preconditioner will be considered. In particular we will compare a diagonal wavelet preconditioner and a more expensive but probably more efficient preconditioner which takes into account the structure of the starting differential operator. This is a joint work with V. Perrier.

KARAGEORGHIS, Andreas (Department of Mathematics and Statistics, University of Cyprus, Cyprus)

Spectral element methods for problems in circular domains

In this paper we discuss the application of spectral methods to problems in circular geometries. This is done by using polar coordinates and approximating with high degree polynomials in each coordinate. In particular, we examine the application of a spectral element method to the solution of Poisson's equation on a disk with discontinuous boundary conditions. The extension of the method to the corresponding Stokes and Navier-Stokes cases is also investigated. This is a joint work with C Bernardi, Analyse Numérique, C.N.R.S. & Université Pierre et Marie Curie, France

MADAY, Yvon (Laboratoire ASCI-CNRS, Orsay France)

Introduction to the mortar element method for high order approximations

The mortar element method is a versatile frame that allows to combine in an easy and optimal way the variational approximations (finite element, spectral element, wavelets..) on a rather general decomposition of the general domain. It is used for a wide number of applications, such as Maxwell equations or mesh adaptivity. The aim of the talk is to present the key arguments of its numerical analysis.

OWENS, Robert (LMF, Ecole Polytechnique Fédérale de Lausanne, Suisse)

An error indicator for mortar element solutions to the Stokes problem

Recently, Bernardi (see C Bernardi, *Indicateurs d'erreur en h-N version des éléments spectraux*, Modél. Math. Anal. Num. **30** (1996) 1-38) derived residual-type error indicators for the spectral element solution to model elliptic problems in 1 and 2 dimensions. Hints were given as to how error indicators of the same type could be derived for the mortar element method in 2 dimensions. Drawing our inspiration from this paper and the work of Bernardi, Métivet and Verfürth (see C Bernardi, B Métivet and R Verfürth, *Analyse numérique d'indicateurs d'erreur*, Publications du Laboratoire D'Analyse Numérique, Université Pierre et Marie Curie R93025 (1993)) and Verfürth (see R Verfürth, *A posteriori error estimators for the Stokes equations*, Num. Math. **55** (1989) 309-325 and R Verfürth, *A posteriori error estimators for the Stokes equations. II. Nonconforming discretizations*, Num. Math. **60** (1991) 235-249), we derive, for the first time, an a posteriori error indicator for mortar element solutions to the Stokes problem. Both planar and axisymmetric cases are considered. Numerical results are given. This is joint work with C Bernardi (Paris) and J Valenciano (Napier, Edinburgh).

PERRIER, Valérie (Laboratoire d'Analyse, Géométrie et Applications, Université Paris Nord, 93430 Villetaneuse, France)

The mortar method in the wavelet context

We present an adaptation of the mortar method in the wavelet context. The idea is to take advantage both on the good approximation properties given by wavelets, and on their ability to provide diagonal preconditioners for elliptic problems.

We consider the Laplace-Dirichlet problem on a rectangular domain, splitted as a union of rectangular, disjoint subdomains. In each subdomain, the discretization is performed with a wavelet space. On each interface, the multiplier space is constructed by "biorthogonalization" of a wavelet trace space. We derive the error estimate, and we present numerical examples. This is a joint work with S. Bertoluzza.

SURI, Manil (University of Maryland Baltimore County, USA)

Optimal convergence rates of hp mortar finite element methods

When mortar methods are used in the context of hp methods, they should possess good convergence properties not only in terms of the mesh size h but also the degree p . Moreover, they should be able to handle highly non-quasiuniform meshes such as *geometric* and *radical* meshes. We consider four different mortaring methods, and show that all of them are robust for non-quasiuniform meshes and lead to exponential hp convergence. Moreover, we present sharp asymptotic convergence rates that depend both on h and p , and show these methods to be well-suited for hp implementation.

This is a joint work with F Ben Belgacem and P Seshaiyer.

ALDROUBI, Akram (Vanderbilt University, USA)

Image processing for diffusion tensor MRI

We construct atomic spaces $S \subset L_2(\mathbb{R}^n, T_1^1)$ that are appropriate for the representation and processing of discrete tensor field data. We give conditions for these spaces to be well defined, atomic subspaces of the Wiener amalgam space $W(C, L_2(\mathbb{R}^n, T_1^1))$ which is locally continuous and globally L_2 . We show that the sampling or discretization operator Dis from S to $l_2(\mathbb{Z}^n, T_1^1)$ is a bounded linear operator. We introduce the dilated spaces $S_\Delta = D_\Delta S$ parametrized by the coarseness Δ , and show that the discretization operator is also bounded with a bounded inverse for any $\Delta \in \mathbb{Z}^n$. This allows us to represent discrete tensor field data in terms of continuous tensor fields in S_Δ , and to obtain continuous representations with fast filtering algorithms.

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FISCHER, Bernd (Institute of Mathematics, Medical University of Lübeck, Germany)

Polynomial wavelets with application to evoked EEG oscillations

In this talk we present a unified approach for the construction of polynomial wavelets. Our main tool are orthogonal polynomials. More precisely, our derivations make use of the general theory of kernel polynomials. Among other properties, the new wavelet scheme enables one to pre-determine the frequency range of the individual levels of decomposition. Several examples illustrate the new approach. In particular, we apply the polynomial wavelet scheme to signals obtained by visual cortex recordings of auditory and visual evoked potentials in the human brain. The obtained results strongly support the suggestion that alpha oscillations in the corresponding EEG are event-related oscillations.

MODERSITZKI, Jan (Medical University of Lübeck, Germany)

On modelling elastic brain deformation

A typical problem of neuro-segmentation in 3D paraffine section spaces is the deformation of the sections due to the building process. We present a linear elasticity model for this kind of deformations. To compute the deformation one needs to solve the so-called Navier-Lamé-equations. A proper discretization of this PDE leads to large linear systems with typically millions of unknowns. Thus, standard direct methods can not be used. However, due to the special structure of the system it is possible to devise a direct method based on Fourier-type techniques. In contrast to most of the commonly used iterative schemes this scheme needs no user supplied parameters. The performance of the presented scheme is demonstrated in a variety of numerical examples, including the computation of brain deformation.

WEICKERT, Joachim (University of Copenhagen, Denmark)

Nonlinear diffusion in medical imaging

Nonlinear diffusion filtering is gaining increasing importance for the preprocessing of digital medical images. This presentation explains the basic principles behind this technique, its theoretical foundation, and it discusses a fast algorithm which has many favourable properties and is well-suited for parallel computers. Recent applications to several medical imaging problems (MRI, 3-D ultrasound, 2-D image sequences) illustrate the potential of nonlinear diffusion filtering.

This is joint work with Karel Zuiderveld, Bart ter Haar Romeny, Wiro Niessen, and Michael Abramoff.

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BOFFI, Daniele (Penn State University, University Park, PA 16802, USA)

Mixed finite elements in the approximation of the eigenvalues of the Maxwell's equations

Our aim is to address some difficulties, as spectral pollution, which arise in computing the eigenvalues of the Maxwell's system by a finite element method. Using an equivalent eigenproblem in mixed form, we propose a criterion to establish whether a finite element scheme is well-suited or not to approximate the eigensolutions and we estimate the rate of convergence for the eigensolutions. Such criterion is based on some properties of the finite element spaces and of a Fortin operator. In particular we apply the above results to the well-known edge elements.

This is a joint work with P. Fernandes, L. Gastaldi and I. Perugia.

CAPATINA-PAPAGHIUC, Daniela (University of Pau, France)

Coupling of primal and mixed finite elements for a parameter-dependent problem

We study a stiff transmission problem, singularly depending upon a small parameter; the model problem considers an elastic body onto which is grafted a highly conductive thin shell. We are interested in its numerical approximation, which may suffer from locking when the parameter tends towards 0. This is actually the case for primal conforming methods. In order to avoid this numerical phenomenon, we employ a primal formulation on the elastic body, coupled with a dual formulation on the thin shell, where locking is expected. For the discretization, we use Lagrange respectively Raviart-Thomas elements, without any interface compatibility for the meshes. The robustness of the method is established and numerical results presented. This is a joint work with J M Thomas.

GATICA, Gabriel N (Departamento de Ingeniería Matemática, Universidad de Concepción, Concepción, Chile)

On the coupling of mixed-FEM and BEM

In this paper we provide some recent results concerning the coupling of mixed finite element and boundary element methods, as applied to several transmission problems in physics and engineering sciences, particularly potential theory and elastostatics. Our analysis includes both primal and dual mixed methods. In addition, we consider linear and nonlinear boundary value problems. We study the different types of variational formulations arising from the coupling procedure and derive results of existence and uniqueness of solution for the continuous and discrete schemes. We also provide a-priori and a-posteriori estimates for the corresponding error. This is a joint work with Salim Meddahi, Jean-Marie Thomas.

MAITRE, Jean-Francois (Equipe d'Analyse Numerique Lyon-St Etienne, CNRS UMR, France)

Relations between mixed, nonconforming finite elements, and finite volumes: Application to a posteriori error estimation for finite volume schemes

For model problems, we have shown, with F.Oudin, that a class of cell-centered finite volume schemes could be obtained from a mixed finite element system; that, using the lowest Raviart-Thomas element, and a mass lumping making trivial the elimination of the vector field. Thanks to this mixed finite element framework, new results have been obtained for finite volume analysis. Our presentation will concern a posteriori estimators, based on the connection between mixed and nonconforming elements (D N Arnold, F Brezzi, T Arbogast, Z Chen), extending results of A Agouzal, F Oudin to rectangular type finite volumes in any dimension, and exhibiting some numerical experiments. This is a joint work with J Baranger, J Olaiz.

MARINI, Donatella (Universita' di Pavia and IAN-CNR, Pavia, Italy)

An analysis of discontinuous Galerkin methods for diffusion problems

We analyze the discontinuous finite element method introduced by Bassi and Rebay, in which a rather peculiar (but quite effective) way of using discontinuous finite elements for diffusive terms has been proposed. We consider as a model problem the Laplace operator in a polygonal domain, in order to cast out the ability of the method to deal with diffusive terms. We rewrite the original formulation in a new and more elegant way, better suited for a mathematical investigation, and show that the original formulation can be rank-deficient when applied to stationary problems. On the other hand, we prove that variants of it are stable and we provide optimal-order estimates. The relationships with mixed finite element formulations are briefly discussed.

TRUJILLO, David (Universite de Pau, France)

Solving drying problem by mixed finite volume method

One may encounter drying problems in many industrial fields. The diversity of the products to be dried involves the development of a large number of techniques of drying. We consider here only the method of thermal drying of porous media. If one regards as principal unknowns, the density of the dry air, the water content and the enthalpy, then one obtains a modeling of the process as a system of three non-linear parabolic equations. The existence of a solution is obtained in a traditional way by a fixed point theorem, while in order to establish the uniqueness we use a transposition method.

The uniqueness of the solution of the initial problem depends then on the existence of solutions of the transposed problem. Finally, we are interested in the approximation of the solution by the means of a mixed finite volume method and we briefly present some numerical results.

TSOGKA, Chrysoula (INRIA, France)

Analysis of a new family of mixed finite elements for elasticity

We present and analyze a new family of mixed finite elements for the velocity-stress formulation of elastodynamics. These elements have two main advantages. First, the symmetry of the stress tensors is satisfied by the approximation space. Second, one can obtain explicit schemes after time discretization, through mass lumping, even in anisotropic media. Obtaining error estimates for this element requires a new abstract theory to overcome two major theoretical difficulties. The first one is due to the fact that the classical discrete Ladyzhenskaya-Babuska-Brezzi conditions are not satisfied. The second one is linked to the treatment of the symmetry condition for the tensors. This is a joint work with Eliane Becache and Patrick Joly.

WOHLMUTH, Barbara (University Augsburg, Germany)

An iterative substructuring method for Raviart-Thomas vector fields in three dimensions

Iterative substructuring methods, also known as Schur complement methods, form one of two important families of domain decomposition algorithms. An iterative method of this kind is introduced for the lowest order Raviart-Thomas finite elements in three dimensions and it is shown that the condition number of the relevant operator is independent of the number of substructures and grows only as the square of the logarithm of the number of unknowns associated with an individual substructure. The preconditioners are then defined in terms of local problems defined on individual substructures and pairs of substructures, and, in addition, a global problem of low dimension. In contrast to standard Lagrange finite elements in 3D the standard coarse space can be used. The results can also be extended to a multi-level, hierarchical basis method; results on its qualitative behavior are obtained by using a strengthened Cauchy Schwarz inequality. The theoretical bounds are confirmed by a series of numerical experiments. This is a joint work with A Toselli and O Widlund.

AINSWORTH, Mark (Strathclyde University, Glasgow, UK)

Domain decomposition for hp-finite element approximations in two and three dimensions

The talk will discuss recent work on developing efficient and practical domain decomposition solvers for *hp*-finite element approximation in two and three dimensions. An overview of the main theoretical results will be presented along with numerical examples illustrating the results.

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CASARIN, Mario A (University of Campinas, Brazil)

Schwarz preconditioners for the spectral element discretization of the steady Stokes equations

The Q^N - Q^{N-2} spectral element discretization of the Stokes equation gives rise to an ill-conditioned, indefinite, symmetric linear system for the velocity and pressure degrees of freedom. We propose a domain decomposition method which involves the solution of a low-order global, and several local problems, related to the vertices, edges, and interiors of the subdomains. The original system is reduced to a symmetric equation for the velocity, which can be solved with the conjugate gradient method. We prove that the condition number of the iteration operator is bounded from above by $C(1 + \log(N))^3/\beta_N$, where C is a positive constant independent of the degree N and the number of subdomains, and β_N is the inf-sup condition of the pair Q^N - Q^{N-2} . We present numerical experiments that validate the theoretical estimates and establish this method as an efficient and theoretically sound iterative scheme for the solution of this saddle point problem. In particular, the iteration count is studied in its relation with the degree of the polynomials and the number of elements, as well as the geometry of the computational domain. If time permits, we will briefly consider the extension of the method for the steady nonlinear Navier-Stokes equation, and its numerical performance.

FISCHER, Paul F (Argonne National Laboratory, USA)

Multilevel overlapping Schwarz methods for spectral elements

We present recent advances in overlapping Schwarz preconditioners for parallel spectral element flow simulations involving millions of gridpoints. Local problems are based upon approximate tensor-product discretizations which admit fast-diagonalization-based solution methods. A coarse-grid solver based upon projection onto a sparse basis attains the minimum possible number of message cycles and significantly shorter messages than competing methods, making it ideally suited to networks of workstations and multi-thousand node teraflops-level machines. An intermediate-scale problem eliminates aspect-ratio limitations of earlier overlapping Schwarz implementations. We illustrate the capabilities of the method for several boundary layer and heat transfer computations at transitional Reynolds numbers.

GUO, Benqi (University of Manitoba, Canada)

Effective preconditioners for the high-order method with Gauss-Legendre-Lobatto interpolation polynomials

The selection of nodal and side modes of shape function is extremely critical to control the condition number of system resulted from high-order method. It requires the essential property: their L^2 -norms are the smallest possible. The Lagrange interpolation polynomials based on GLL points give this property, and they are easy to be understood in analysis and implemented in computation. The usage of these shape function has successfully leads to the optimal polylogarithmic bounds of preconditioners for the spectral and finite/boundary element method in three dimensions.

HEUER, Norbert (Universität Bremen, Germany)

Preconditioners for high order boundary element systems

We deal with the p and h - p versions of the Galerkin boundary element method for first kind integral operators on surfaces. The arising linear systems are fully occupied and ill-conditioned. We present preconditioners which are based on decompositions of the ansatz spaces. For operators of order one continuous ansatz functions are required. Here, the analysis is carried out within $H^{1/2}$ which is the trace space of H^1 . On the other hand, the energy space of operators of order minus one is the dual space of $H^{1/2}$ and continuity of the trial functions is not needed. The efficiency of the proposed methods is demonstrated by numerical experiments.

KATZ, I Norman (Washington University, St Louis, Missouri, USA)

Multi-p processes and pre-conditioners

A natural analogy to the multi-grid method which is based on the h -version of the finite element method is the multi- p method which is based on the p -version and hierarchic basis functions. Multi- p processes, including standard V-cycles, modified V-cycles, varying V-cycles, and fully multi- p methods, can be used as pre-conditioners. Methods for enhancing the performance of multi- p preconditioners by parallelization or replacing Gauss-Seidel smoothers with damped Jacobi smoothers are described. Results of numerical experiments are presented. This is joint work with Xian-Zhong Guo, Washington University, and Ning Hu, Endocardial Solutions Inc., St. Paul, Minnesota.

PATRA, Abani K (State University of New York, USA)

On the development of domain decomposition solvers for adaptive hp finite element methods

Adaptive hp finite element methods provide very efficient discretizations for a wide class of problems. Two level iterative substructuring and coarse grid type preconditioning methods provide efficient parallel solution algorithms for the poorly conditioned irregularly sparse linear systems arising from these grids. We report further progress in this area. We describe the use of these solvers as inner solvers for either inexact Newton methods for non-linear problems and/or as part of an implicit time integrator for transient problems. Numerical studies, proofs of convergence and bounds on performance for these solvers are also presented.

SHERWIN, Spencer J (Imperial College, UK)

Low energy basis preconditioning for unstructured spectral/ hp element methods

We consider an hp discretisation of the Navier-Stokes equations in three dimensions, as applied in the unstructured solver Nektar. After applying a time discretisation which decouples the viscous and inviscid parts of the operator, the most computationally intensive part of the solver are a series of three elliptic solves, one Poisson solve and three Helmholtz solves, which are performed at each time step. Each of these elliptic solves is preconditioned with an iterative substructuring type domain decomposition method, which takes advantage of the natural splitting of the basis into interior, face, edge, and vertex basis functions. As noted by several authors, special care must be taken in three-dimensions in order to produce a method which is scalable with respect to h and p . In particular, we propose a set of numerically evaluated low-energy basis functions calculated by solving a local elliptic problem on a regular reference element which is then mapped onto the global elements that constitute the solution mesh. The resulting method is quasi-optimal in terms of iteration count and is computationally efficient due to its local construction. In addition we will demonstrate the efficiency of the method in a set of numerical experiments. In particular we will show that for the solution of a standard Poisson equation the low-energy preconditioner significantly reduced the number of iteration counts as well as producing a factor of three improvement in the computational solve time.

WARBURTON, Timothy (Oxford University, UK)

Overlapping Schwarz preconditioners for solving elliptic problems on polymorphic/ hp elements

Over the past few years we have been developing spectral/ hp methods on unstructured, mixed element grids for CFD in the research code Nektar. Recently we have looked at ways of speeding up our elliptic preconditioned conjugate gradient solver using an overlapping additive Schwarz preconditioner. We will present numerical evidence that the preconditioned Helmholtz operator has a condition number bounded independently of the polynomial degree vector and h -refinement. We will also show that this holds for both the Schur complement and the fully iterative approach to inverting this operator.

DAWSON, Clint (University of Texas at Austin, USA)

Upwind-mixed and local discontinuous Galerkin finite element methods for ground-water transport problems

In recent years, methods for advection-diffusion equations based on combining upwinding techniques with some type of finite element approach have been developed and implemented. In this talk, we will focus on two such methods, one based on combining upwinding with a mixed finite element method for diffusion, and another based on applying a discontinuous Galerkin method. Theoretical error estimates for both methods will be discussed as well as their application to contaminant transport problems. Moreover, the combination of these methods with dynamically adaptive meshes will also be presented.

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ESPEDAL, Magne (Department of Mathematics, University of Bergen, Bergen, Norway)

Finite volume based local grid refinements for simulation of multiphase flow in fractured reservoirs

Flow in hydrocarbon or groundwater reservoirs is commonly influenced by fracture systems, which may either enhance or depress permeability. Often the fracture system control the flow pattern in a reservoir. This emphasizes the need to include spatial distribution of fractures and to understand and evaluate the flow characteristics at all scales. The work is based on a three dimensional, multi-component and three phase model allowing for changing reservoir geometry like compaction. The model is discretized by a finite volume method. General local grid refinements based on domain decomposition, is implemented. Numerical results for flow in a fractured reservoir model, consisting of different sediments, will be presented.

JAFFRÉ, Jérôme (INRIA-Rocquencourt, France)

Mixed-hybrid finite elements for two-phase flow in porous media with two rock types

Mixed-hybrid finite elements provide a rigorous framework to generalize standard cell-centered finite volume methods. They are locally mass conservative methods and they use cell and edge unknowns. Therefore these methods are convenient to approximate interface problems, while respecting closely all physical assumptions. The method will be illustrated with the problem of modeling incompressible two-phase flow in a porous medium with two rock types. On the interface between subdomains with different rock types, writing physical conditions - conservation of each phase and continuity of the phase pressures - leads to nonstandard interface conditions. Numerical results will be shown. This is joint work with J E Roberts and Wang Xuewen from INRIA-Rocquencourt.

SCHNEID, Eckhard (University of Erlangen-Nuremberg, Germany)

Stability of an adaptive mixed finite element discretization of saturated-unsaturated flows in porous media

Richards equation is a suitable model for saturated-unsaturated groundwater flow. This elliptic-parabolic degenerate partial differential equation is discretized with hybridized mixed finite elements. The resulting system of nonlinear equations is solved by Newton's method and multigrid algorithm. The mixed fem discretization exhibits oscillations if sharp fronts are occurring. We consider monotonicity of the discrete problem and grid refinement to prevent this. Water redistribution involves timescales at different orders of magnitude. We introduce an adaptive strategy to control time step sizes following the timescale of water redistribution in a reasonable way.

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CALVETTI, Daniela (Case Western Reserve University, USA)

Expansion methods in image restoration

Restoration of images degraded by blur and noise gives rise to very large, severely ill-conditioned linear systems of equations. The solution of such linear systems requires that some form of regularization be applied to avoid disastrous amplification of the noise. This is usually carried out by means of filter functions, which adjust the amount of regularization applied to the problem according to the properties of the blurring operator and the amount of noise in the degraded image. In the present talk we describe regularizing iterative methods based on the expansion of filter functions into orthogonal polynomials. The methods described determine a suitable value of the regularization parameter in an adaptive fashion under different assumptions regarding the noise.

CHAN, Tony F (University of California at Los Angeles, USA)

Nonlinear PDE models in image processing

PDE models and methods in image processing have emerged recently as an alternative to traditional transform and statistically based methods. The PDEs are designed to possess certain desirable geometrical properties and part of the motivation is a more systematic approach to restoring images with sharp edges, as well as for image segmentation. The PDE formulations calls for new computational techniques which are different from the traditional frequency domain and algebraic approaches. Among the computational difficulties are the highly nonlinear and singular nature of the PDEs that arise and the need to invert ill-conditioned nonlinear differential-integral operators efficiently. In my talk, I will give an introduction to this field after which I will highlight work in our group on the development of efficient numerical methods, as well as new models for multi-spectral and color images, blind deconvolution, segmentation and active contours, etc.

MIKULA, Karol (Slovak University of Technology, Slovakia)

Nonlinear multiscale analysis of 3D image sequences

We will discuss models and numerical methods for multiscale analysis of space-time images. Nonlinear partial differential equations are used either for analysis of static frames or for processing of the time sequence considering spatial as well as temporal coherence. In the present talk we will describe adaptive finite element and finite volume methods for solving the regularized Perona-Malik anisotropic diffusion equation and geometrical equations of mean curvature flow type used for spatial diffusion process in static frames. The idea of movie multiscale analysis of Alvarez, Guichard, Lions and Morel combined with geometry driven spatial diffusions is then used for processing of the image sequences. Computational results with artificial, real (echocardiographic) images and video simulations of image analysis will be presented and discussed.

SETHIAN, James A (University of California at Berkeley, USA)

Application of fast marching and level set methods to image processings and computer vision

We will discuss the application of Fast Marching Methods and Level Set Methods to Image Processing and Computer Vision. Fast Marching Methods (Sethian, 1996) and level set methods (Osher and Sethian, 1988) are computational techniques for tracking the evolution of fronts moving under complex speed laws. They both grew out of the earlier theory of curve and surface evolution (Sethian 1982, Sethian 1985). This talk will contain a brief review of these methods, followed by a description of some of the most recent computational and algorithmic advances in their application to computer vision and image analysis. This will be followed by the application of these techniques to problems in shape segmentation, medical imaging, offsetting, shape recognition and shape analysis. We will provide a large number of examples, including those from CT, MRI, EBT scans, and CAD/CAM issues.

BELL, John B (Lawrence Berkeley National Laboratory, Berkeley, USA)

Block-structured adaptive mesh refinement for incompressible flow

We describe an adaptive projection algorithm for low Mach number flows. The basic approach uses hierarchical grids that are refined in both space and time. In this presentation we will review the single grid projection methodology and discuss the key issues in the algorithm that must be addressed in developing an adaptive algorithm. With these issues in mind, we discuss the design principles that we use to solve partial differential equations on adaptive grids. We then describe how these principles are used to develop an adaptive version of the projection algorithm. Numerical examples illustrating the capabilities of the method will be presented.

LIU, Jian-Guo (Mathematics, University of Maryland, USA)

Gauge method for viscous incompressible flows

We explore the gauge formulation of the incompressible Navier-Stokes equation in terms of an auxiliary field that differs from the velocity by a gauge transformation. The gauge freedom allows us to assign simple and specific boundary conditions for both the auxiliary field and the gauge field, thus eliminating the issue of pressure boundary condition in the usual primitive variable formulation. Although it closely resembles the projection method, the gauge method has the advantage that the gauge Poisson equation (GPE) in the projection step can be solved by standard Poisson solvers including the five-point formula. This is in contrast to the projection method in which the pressure Poisson equation (PPE) has to be solved using special Poisson solvers. We also give applications to non-local variational problems.

MINION, Michael (Applied Mathematics, University of North Carolina, USA)

Consistent no-slip boundary conditions for pressure increment projection methods

Projection methods have become one of the most popular grid based methods for problems involving the simulation of incompressible flows. Of the many varieties of projection methods, pressure increment schemes are very common. These methods update the pressure using the gradient portion of the Hodge decomposition of an intermediate (i.e. non-divergence free) velocity update. When the velocity update is calculated semi-implicitly, boundary conditions for this update and the subsequent projection must be determined. The usual manner in which this is done leads to a pressure boundary error which has been well documented but is still misunderstood. We will present consistent boundary conditions for pressure increment schemes which remove the boundary layer error. We will also draw analogies between these boundary conditions and those used in vorticity and gauge variables. This is a joint work with David Brown, Lawrence Livermore National Lab and Ricardo Cortez, Tulane University.

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TUREK, Stefan (Institute for Applied Mathematics, University of Heidelberg, Germany)
Multilevel pressure Schur complement techniques for the incompressible Navier-Stokes equations

On the basis of the MPSC techniques ("Multilevel Pressure Schur Complement") we have recently derived a general solution framework for discretized incompressible flow problems which includes most of existing approaches (projection schemes, pressure correction schemes, SIMPLE-like techniques, Vanka smoother, etc.). We show how those "classical" methods can be essentially improved with respect to robustness and efficiency; hereby even exploiting the high performance of modern computer platforms. Together with appropriate discretization tools and adaptive mechanisms, the quality of CFD tools can be significantly improved.

WETTON, Brian R (Mathematics, UBC, Canada)
Error analysis of methods for incompressible flow

The purpose of this talk is two fold. First, it will serve as an introduction to the mini-symposium, "Time stepping for viscous incompressible flow: state of the art and new ideas". The main challenges, theoretical and practical, of developing computational methods for incompressible flow will be outlined. In the second part of the talk, my own work on the error analysis of pressure increment schemes will be presented.

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DUCHATEAU, Paul (Colorado State University, USA)
The abstract structure of coefficient-inverse problems

The identification of unknown coefficients in parabolic partial differential equations from various types of overspecification produces a class of problems with a well defined abstract structure. Using abstract integral identities, it is shown that each identification problem is associated with a unique dual problem. The identification problem is then shown to be solvable if the dual problem is controllable; (the overspecification on which the identification is based determines the control in the dual problem). Not only are the techniques useful for proving the identifiability of certain coefficients, they also provide information that may be useful for improving design of identification experiments. These results are illustrated for some examples of identifications relating to flow and transport in porous media.

GOTTLIEB, Johannes (University of Karlsruhe, Germany)
Hysteresis identification for porous media flow

The paper deals with modeling of hysteretic behaviour of flow in partially saturated porous media. We compare different hysteresis models and corresponding hysteresis identification procedures. A numerical scheme is discussed for the Duhem hysteresis model.

KNABNER, Peter (University of Erlangen-Nuremberg, Germany)
Identifiability of adsorption characteristics in porous media flow and experiment design

The displacement velocity of solutes in e.g. the underground or in chromatographic devices is strongly influenced by sorption processes. Sorption isotherms or rate functions which describe the process and enter into the transport model as nonlinearities, usually have to be determined indirectly by breakthrough experiments. Based on an abstract version of the method of integral identities, we prove identifiability of the unknowns for various situations and experimental setups. In cases, where the method is inconclusive, it gives hints how to change the experiment design appropriately.

SPIVACK, Mark (University of Cambridge, UK)
Identification of source term in a coastal evolution equation

The paper derives a method for the reconstruction of a source term in a linear parabolic equation, describing seabed evolution over long time scales. The approach is based upon inversion of the widely-used split-step solution for the direct problem, and assumes that data is available on a regular grid at successive time steps. This is applied to measurements gathered at intervals over 150 years for a group of sandbanks near East Coast of the UK. The application to statistics and prediction of coastal movement will be discussed. This is a joint work with D E Reeve.

BEWLEY, Thomas R (Department of MAE, UC San Diego, USA)

Application of linear feedback to nonlinear problems in fluid mechanics

This paper examines the application of linear optimal control theory to a low-order nonlinear chaotic convection problem. Linear control feedback is found to be fully effective only when it is switched off while the state is far from the desired equilibrium point, relying on the attractor of the system to bring the state into a neighborhood of the equilibrium point before control is applied. Linear estimator feedback is found to be fully effective only when *a*) the Lyapunov exponent of the state estimation error is negative, indicating that the state estimate converges to the uncontrolled state, and *b*) the estimator is stable in the vicinity of the desired equilibrium point. The aim in studying the present problem is to understand better some possible pitfalls of applying linear feedback to nonlinear systems in a low-dimensional framework. Such an exercise foreshadows problems likely to be encountered when applying linear feedback to infinite-dimensional nonlinear systems such as turbulence. It is important to understand these problems and the remedies available in a low-dimensional framework before moving to more complex systems such as turbulence.

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CHOI, Haecheon (Department of Mechanical Engineering, Seoul National University, Korea)

Suboptimal feedback control of vortex shedding

The objective of this study is to develop a systematic method of controlling vortex shedding behind bluff bodies using control theory. A suboptimal feedback control algorithm is applied to flows around a circular cylinder (to decrease drag) and an airfoil (to increase lift). The location of sensors is limited to the wall and control inputs are the blowing and suction on the wall. Several cases have been numerically simulated to investigate the performance of the control algorithm. Most cases considered show that vortex shedding can be successfully controlled using the suboptimal feedback control procedure.

COLLIS, S Scott (Rice University, Houston, Texas, USA)

Large eddy simulation of active turbulence control

Advances in high-performance computing and Large-Eddy Simulation (LES) have made it possible to obtain accurate solutions of complex, turbulent flows at moderate Reynolds numbers. With these advances, computational modeling of turbulent flows in order to develop, evaluate, and optimize active control strategies is feasible. This talk will present approaches to numerical modeling of opposition control and optimal control of turbulent channel flow with attention to algorithms that utilize the dynamic subgrid-scale LES model. Approximately 25 percent drag reduction is achieved by opposition control using LES, which is in good agreement with previous DNS results. The optimal control scheme based on LES has been successfully implemented and LES results will be compared to prior DNS results for optimal control of terminal turbulent kinetic energy. The agreement between LES and DNS indicates that reliable flow control strategies can be efficiently developed based on LES models and extensions of the current approach to more complex flows will be discussed.

HINZE, Michael (Karl-Franzens Universität Graz, Austria and Technische Universität Berlin, Germany)

Constructing feedback laws for fluid flows

Two approaches for obtaining closed-loop control laws for fluid flows are presented. **Instantaneous control** The Navier-Stokes equations are discretized w.r.t. time. At each time step (or at selected time steps) an optimization problem with an instantaneous cost function is solved approximately. **Reduced Order Modeling** The solution of the Navier-Stokes equations is approximated using the snapshot proper orthogonal decomposition method proposed by Sirovich or the reduced basis method. A minimization problem is formulated that involves the reduced Navier-Stokes equations as subsidiary conditions. Among other things a feedback synthesis is developed for the reduced system. The effectiveness of the approaches is illustrated at the construction of control laws for the backward facing step flow and the flow around a cylinder in two spatial dimensions.

KAUFFMANN, Andreas (Technische Universität Berlin, Germany)

Control of fluid flow using reduced order models

A general approach for obtaining suboptimal control laws for fluid flows is presented. The Navier Stokes equations (NSE) are approximated using a Galerkin Ansatz with basis functions generated from snapshots of solutions of the NSE. This results in a low-dimensional dynamical system which is then used instead of the NSE as a subsidiary condition in the optimization process. The optimal controls of the reduced approach are used as suboptimal open loop control for the NSE. Furthermore a feedback synthesis based on given sets of the reduced system is presented. The effectiveness of the methods is demonstrated with several numerical examples.

MARDUEL, Xavier (SFB Optimierung und Kontrolle, Karl Franzens Universität, Graz, Austria)
Sub-optimal control of transient non-isothermal viscoelastic fluid flows

Sub-optimal control of viscoelastic fluid flow in a 4 to 1 contracting channel is investigated. The control mechanism is based on heating or cooling the fluid along a portion of the boundary of the flow domain. A non-isothermal model for viscoelastic fluids is used consisting of the so-called Phan-Tien-Tanner model with relaxation time and elastic viscosity depending on temperature. The goal of the control is to find a temperature on the boundary of the domain such that the large recirculation zones at the corners of the contracting channel are reduced and the fluid behaves like a viscous one.

TEMAM, Roger (Indiana University, Department of Mathematics, USA)
Robust control of Navier Stokes equations

It is useful for many industrial applications to be able to control turbulence in fluid flows; in general the purpose is to reduce turbulence (e.g. in aeronautics), but in some cases it is desirable to increase it (mixing and combustion). From the theoretical point of view the problems that we face are problems related to Navier-Stokes equations, to calculus of variations and to the control of nonlinear systems; from the practical viewpoint the problems encompass also the modeling of the control problem and the numerical simulation of turbulent flows. In the first part of the lecture we will recall results on the optimal control of turbulent flows, addressing such questions as the modeling of the problems, the existence of an optimal control and its approximation (joint work with F Abergel). Robust control concerns the control of a system in the presence of unpredictable disturbances; the purpose is to keep the system under control in the case of the worse possible disturbance. We show how to formulate this problem for fluid flows in the context of calculus of variations and convex analysis. Then, under suitable conditions, we establish the existence and uniqueness of an optimal state, and we give some indications on its approximation. This is a joint work with T Bewley and M Ziane.

VOLKWEIN, Stefan (Institut für Mathematik, Karl-Franzens Universität Graz, Austria)
Approximations of optimal control problems by proper orthogonal decomposition

The proper orthogonal decomposition (POD) is a method to derive reduced order models for dynamical systems. The close connection between POD and singular value analysis is discussed. POD is utilized to solve open and closed loop optimal control problems for linear and nonlinear partial differential equations. Where it is possible POD-based algorithms are compared with numerical results obtained from finite element discretizations.

DOLD, John W (UMIST, UK)
Flame ball stability in a dusty gas

A reactive-diffusive model for flame-balls is considered, incorporating thermally-sensitive exothermic chemistry restricted to a thin flame-sheet, heat losses, and the presence of an inert non-mobile constituent in the medium. This "inert dust" is only taken to influence the model equations via its heat-capacity, as an additional, homogeneously distributed phase, exchanging heat with the reacting gas-phase. Steady solutions are unaffected, but their stability is significantly altered in a manner which is, effectively, equivalent to reducing the Lewis number of the chemical reactants. This finding has some implications for the safety of dusty explosive gases in the possible presence of localised heat sources.

GOL'DSHTEIN, Vladimir (Ben Gurion University, Israel)
Flame propagation in multiphase media

The aim of the present paper is to study the influence on the flame propagation in the combustible gas mixture of an addition of the liquid or/and the solid phase. In this situation the flame structure becomes more complicated including possible temperature decreasing ahead or/and behind the reaction zone. It can lead also to the essential reduction of the flame speed.
 This is a joint work with Ann Zinoviev.

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KUZMENKO, Grigory (Ben-Gurion University of the Negev, Israel)

Thermal explosion in sprays

The effect of a flammable spray on thermal explosion in a combustible gas mixture is investigated. A suggested simplified model contains the essentials of the basic physical processes at work. The adopted approach is based on application of the integral (invariant) manifold method. The dynamical behavior of the system is classified. It is demonstrated that three main possible types of behavior can be identified: slow regimes, the conventional fast explosive regimes and delayed explosive regimes. Parametric regions of an existence of these regimes are determined and dynamical characteristics of the regimes are studied.

SHCHEPAKINA, Elena (Samara State University, Russia)

Canards and black swans in combustion

Two-temperature models of combustion under taking into account gas consumption and heat losses from reactant phase are investigated. The case of uniform temperature distribution and phase-to-phase heat exchange is considered. The models represent the three-dimensional singularly perturbed systems of ODE. Canard type trajectories are used to modelling of critical regimes and calculation of critical conditions of self-ignition. The slow integral manifolds with changing stability named black swans are used to construct feedback control guaranteeing a safe high-temperature regime of combustion.

SOBOLEV, Vladimir A (Samara State University, Russia)

Travelling waves of canard type

The paper is devoted to the phenomenon of flame propagation in a combustible gas in the case of autocatalytic reaction under taking into account the thermal conductivity and the reaction substance diffusion. The new class of travelling waves - waves of canard type is described and studied using the integral manifolds method for singularly perturbed systems. The canard (or French duck) is a specific trajectory of singularly perturbed ODE systems with stable and unstable slow parts. It is shown that the two-dimensional ODE system with automodel independent variable possesses a canard heteroclinic trajectory and the corresponding value of travelling wave velocity is calculated.

This is a joint work with Klaus Schneider, WIAS, Berlin.

ABABOU, Rachid (Institut de Mécanique des Fluides de Toulouse, France)

Stochastic velocity-pressure fields in random porous media: Statistical expansions, solutions, and homogenization.

This paper presents a mathematical analysis of Darcy flow in randomly heterogeneous porous media, with multi-dimensional and statistically anisotropic random field properties, such as permeability $K(x,y,z)$. The case of single-phase steady-state flow is analyzed in detail. The spatial-statistical properties of the flow are determined based on (1): a formulation of the stochastic flow equations directly in terms of velocity (or areal flux density); and (2): a formal expansion of these equations in terms of the amplitude parameter "sigma" (standard deviation of $\ln K$). It has been shown that such expansions are convergent in the 1-D case (Ababou 1995). Here, a first-order perturbation solution is presented in terms of the random velocity vector field (variance, spectral density) for statistically anisotropic porous media with arbitrary orientation of principal axes with respect to mean velocity. Moreover, the permeability homogenization problem (upscaling) is recast as a resistivity homogenization problem, and the two approaches are compared. Finally, new extensions of this approach to statistically inhomogeneous problems and to transient two-phase flow systems are introduced and discussed.

JURAK, Mladen (Department of Mathematics, University of Zagreb, Croatia)

Scaling up two-phase flow in porous media: comparison of methods

Mathematical homogenisation based on conservation of orders of different energies (capillary, viscous, kinetic) can give an answer to the problem of upscaling from "geological grid" (fine scale) to "numerical grid" (coarser scale). However, the form of the nonlinearities in two-phase flow equations is not necessary conserved after change of scale. Thus, the homogenisation method search for a phenomenological description of the reservoir at the "coarser scale" that is, under certain flow conditions, of the same form as the one at the "fine scale". We present here an implementation of the upscaling method based on the mathematical homogenisation, developed by A Bourgeat and A Hidani, and we make a comparison with the classical upscaling methods of petroleum engineering. This is a joint work with A Bourgeat.

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PANFILOV, Mikhail (Russian Academy of Sciences; Moscow Lomonosov University, Russia)

Macroscale nonlocality in flow through highly heterogeneous media

Nonstationary Darcy's flow of single-phase and two-phase fluids through highly heterogeneous media is studied using homogenization methods. Arising of macroscale phenomena, nonlocal in the time, is the basic effect caused by high heterogeneity. For single-phase system, nonlocal macroscale Darcy's law is deduced, with the kernel of the integral operator explicitly defined. In case of two-phase flow, the similar modification of Darcy's law is deduced too, but the relaxation correction includes a characteristic time dependent on saturation. Numerical simulation of the cell problems has been performed to study the structure of the relaxation times and integral kernels. Results obtained allow to compute dynamic effective relative permeabilities and capillary pressure for double porosity media.

QUINTARD, Michel (Institut de Mécanique des Fluides de Toulouse, France)

Two-phase flow of binary mixtures in homogeneous and heterogeneous porous media

Generalized dispersion equations are usually introduced to describe the flow of several components and phases through porous media. In this paper, this model is discussed based on results obtained from the method of volume averaging, coupled with pore-scale simulations of multiphase flow. We focus on a two-phase system with two components, one being at a dilute concentration (tracer). Macroscopic equations are obtained, and several local closure problems are provided that allow to calculate dispersion tensors and other properties from pore-scale geometry, velocities, and fluid characteristics. The solutions of these closure problems are provided in the case of representative unit cells in 2-D. The two-phase flow equations are solved by using a boundary element technique.

Dispersion tensors are then calculated by solving the closure problems associated with the dispersion equations using a finite volume formulation of the PDE's. The results show the strong influence of geometry, velocity and saturation on the effective parameters. They are extended to a larger scale including the effect of heterogeneities. A preliminary result is obtained in a special case corresponding to single-phase flow at maximum saturation. A new large-scale dispersion equation is derived, with a macro-dispersion tensor that can be determined from the heterogeneity through a set of closure problems. Finally, a more general result is obtained for a quasi-static two-phase flow problem.

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BRUEL, Dominique (Centre D'informatique Géologique - Ecole des Mines de Paris - Fontainebleau - France)

Use of stochastic fracture network models for the flow problem

Due to tectonic history, hard rock exhibit heterogeneous fracture distribution patterns, that include all the possible length-scales. As a result, connectivity is often scale dependent and equivalent continuous media may be inappropriate to represent flow. Discrete Fracture Network models are aimed at understanding these specific difficulties. The properties of individual fractures are randomly and independently generated, inferred from statistical analysis of in-situ data records. An example, including the calibration of the hydraulic properties of the fractures against local hydraulic tests is discussed. Valuable results are obtained when modelling the global flow into a gallery and when predicting pore pressure changes in the rock in response to a pressure wave at the walls.

JAFFRÉ, Jérôme (INRIA-Rocquencourt, France)

Domain decomposition for flow in a fractured porous medium

We are concerned with the numerical modeling of flow in a fractured porous medium, particularly in the case where the fractures are large enough to be modeled individually. These fractures are considered themselves to be a porous medium with large permeability and are represented as $(n-1)$ -dimensional objects for a problem in n dimensions. The domain is divided by these fractures into subdomains separated by interfaces with nonstandard transmission conditions. Then the flow is calculated via domain decomposition. Numerical results will be shown. This is a joint work with Clarisse Alboin and Jean E Roberts of INRIA-Rocquencourt, France and Christophe Serres of IPSN, France

PANFILOV, Mikhail (Russian Academy of Sciences, Oil & Gas Research Institute; Russia)

Effective flow in highly heterogeneous disordered media: Homogenization and numerical analysis

Two approaches are developed to deduce averaged models of flow in disordered porous media. The first is based on the methods of quantum field theory and Feynmann's diagram technique. The kernels of averaged equations, called as mass operators, constitute some functional of the correlation functions of all orders. A modification of this method is developed for highly heterogeneous media. In this case, the mass operators can not be simplified to any local forms. The second approach is based on asymptotic two-scale methods of homogenization. The basic problem of disordered media is solved, how to determine the heterogeneity scale when each cell problem becomes independent of other cells. For a medium with thin highly permeable fractures, exact analytical results are obtained. This is a joint work with Yuri Kukharenko and Pavel Kukharenko of the Russian Academy of Sciences, Institute of the Earth Physics.

BAI, Zhaojun (University of Kentucky, Lexington, USA)

Adaptive error estimation of reduced-order modeling of linear dynamical systems via Krylov-subspace techniques

Krylov-subspace based techniques, such as PVL and PRIMA, have emerged as popular tools for reduced-order modeling of linear dynamical systems. In practical applications of these techniques, it is important to have an effective error estimation on the approximations of the original system by the reduced-order one. In this talk, we will discuss several approaches for the error estimation in both frequency and time domains. We will also examine the practicality of these approaches for developing efficient adaptive error estimators. A number of examples on applying these approaches to linear circuit systems will be presented.

FREUND, Roland W (Bell Laboratories, Lucent Technologies, Murray Hill, USA)

Passive reduced-order modeling for VLSI interconnect analysis

The performance of VLSI circuits is increasingly dominated by the effects of the wires connecting the circuit cells, the so-called interconnect, and therefore, the interconnect needs to be included in numerical simulations of the circuit. The current state-of-the-art is to describe the interconnect by huge RLC networks that are then replaced by much smaller reduced-order models generated via Krylov-subspace methods. To guarantee stability of the overall simulation, it is crucial that the reduced-order models inherit the passivity of the RLC network. In this talk, we describe variants of Krylov-subspace methods that generate, both in theory and practice, passive reduced-order models.

NUNNARI, Giuseppe (Università di Catania, Catania, Italy)

Reduced-order modeling by non-integer order equations

Non-integer order systems has been studied by several authors to model particular physical systems (electrical, biological etc.). In particular it can be shown that a non-integer order system is equivalent to an infinite-order LTI systems. This feature can be considered useful for model-order reduction purposes. The main aim of this talk is to show the mathematical background of this new approximation theory, the criteria for selecting the order of a non-integer order model which behaves as the original integer-order ones, and the quality indexes that can be considered for assessing the goodness of the approximated model. Some examples and simulations will be reported.

This is joint work with L Fortuna, G Muscato, and D Porto.

PHILLIPS, Joel R (Cadence, San Jose, USA)

Model-extraction technology for RF communications systems analysis

Incorporation of component nonidealities in high-level design of RF communications systems requires efficient extraction of compact models from detailed nonlinear circuit descriptions. Circuit components of RF systems exhibit frequency conversion effects and so are modelled as time-varying linear elements. By use of an approximate Krylov-subspace projection formalism, algorithms for model reduction of time-varying systems can be efficiently incorporated in a general-purpose circuit simulation tool. The Krylov-subspace based algorithms can be used to generate time-domain descriptions of circuit input-output behavior, as well as of stochastic effects such as noise.

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RUHE, Axel (Chalmers University of Technology, Göteborg, Sweden)

Rational Krylov algorithms for eigenvalue problems and model reduction

Rational Krylov is an extension of the Lanczos or Arnoldi eigenvalue algorithm where several shifts (matrix factorizations) are performed in one run. We will show how Rational Krylov can be used to find a reduced-order model of a large linear dynamical system. In Electrical Engineering, it is important that the reduced model is accurate over a wide range of frequencies, and then Rational Krylov with several shifts comes to advantage. We will also show that the reduced model is stable and passive, whenever the full system is, provided certain precautions are taken. Numerical examples will be demonstrated.

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BUFFA, Annalisa (University of Pavia, Italy)

The mortar element method for the 2D and 3D simulation of Maxwell's equations

Since most of simulations in electromagnetism are computationally expensive, a good performing domain decomposition method is of high interest. We propose a domain decomposition method based on the discretization of Maxwell's equations via finite elements of Nedelec's type in both 2D and 3D case. Nonmatching grids at the interfaces are allowed and the coupling among domains is done by means of a space of Mortar functions. The resulting method is nonconforming in the whole domain and conforming in each sub-domain. We detail the construction of the Mortar spaces and of the nonconforming approximation spaces in both 2D and 3D case; we discuss the optimality of the error estimates and we present some applications.

HOPPE, Ronald H W (Institute of Mathematics, University of Augsburg, Germany)

Adaptive mortar edge element methods in the computation of eddy currents

We are concerned with domain decomposition methods on nonmatching grids for the numerical solution of interior domain problems associated with the quasistationary limit of Maxwell's equations. Starting from a macro-hybrid variational formulation with respect to a nonoverlapping decomposition of the computational domain, we consider a mortar approach based on individual edge element discretizations of the subdomain problems and the realization of weak continuity constraints for the tangential traces on the skeleton of the decomposition. Emphasis will be laid on the iterative solution of the resulting saddle point problem and on local adaptive refinement by means of an efficient and reliable a posteriori error estimator.

MAGOULÈS, Frédéric (Office National d'Études et de Recherches Aérospatiales, France)

A method of finite element tearing and interconnecting for the Maxwell equations

We present a Lagrange multiplier based domain decomposition method for solving iteratively large-scale systems of equations arising from the discretization of high-frequency exterior Maxwell problems.

The proposed method relies on two key ideas: (1) the elimination of local resonance via the stabilization of each subdomain operator by a complex interface mass matrix associated with intersubdomain radiation conditions; (2) the use of a global preconditioner constructed using a coarsening theory for filtering low frequency errors and accelerating convergence.

When equipped with the global preconditioner, the performance of the proposed method becomes insensitive to the mesh size, frequency range and number of subdomains.

RAPETTI, Francesca (ASCI, CNRS, France)

Simulating Eddy currents distributions by a finite element method on moving non-matching grids

The computation of the space and time distribution of the induced currents in electromagnetic systems is of great importance for performance predictions and devices design. The subject of our research activity is the analysis and development of simulation tools to effectively predict the induced currents distribution in non-stationary geometries with sliding interfaces. As an example, we have studied a system composed of two solid parts: a fixed one (stator) and a moving one (rotor) which slides in contact with the stator. Our research starts from a two dimensional mathematical model based on the transverse magnetic formulation of the eddy currents problem in the time domain. The approximation of the problem is based on a mortar method combined with the linear finite elements discretization in space and the implicit first order Euler scheme in time. After a brief introduction of the problem, we focus our attention on the numerical results.

WIDLUND, Olof B (Courant Institute, USA)

Schwarz Methods for $H(\text{div})$ and $H(\text{curl})$ finite element problems

New domain decomposition methods for finite element methods of Raviart-Thomas and Nédélec type, which are used to approximate elliptic operators of divergence type and Maxwell's equation, are introduced. Both iterative substructuring methods and two-level overlapping Schwarz methods are included. Results of numerical experiments and some of the ideas underlying the proofs will be discussed. This work, which has required the extension of previously known technical tools in several directions, has been carried out jointly with Barbara Wohlmuth of Augsburg, Germany, and Andrea Toselli of the Courant Institute.

ISHIMURA, Naoyuki (Department of Mathematics, Hitotsubashi University, Kunitachi, Tokyo, Japan)

A crystalline motion of spirals

Modern physics theories claim that the dynamics of interfaces between the two-phases is described by evolution equations involving the curvature and various kinematic energies. If the interfacial energy has the convexified Frank diagrams that are polygonal, which is referred to as the crystalline energy, then the motion of polygonal interfaces is explicitly given and deserves a mathematical model of the dynamics of real crystals.

We consider the evolution of spiral-shaped polygonal curves by their crystalline curvature. Exploiting the comparison argument, we prove the local existence and uniqueness of the motion. For the curves with symmetry, we show that its evolution can be traced beyond singularities.

NOVAGA, Matteo (Scuola Normale Superiore, Pisa, Italy)

Facet-breaking for 3D crystalline curvature flow: Mathematical aspects

Evolution of interfaces by the so-called crystalline curvature has been deeply investigated in the past, and the behaviour is basically well understood for the evolution of polygonal curves in two dimensions, at least in the case of zero external forces, or when the external forces are independent of space. On the contrary, the evolution of 3D faceted surfaces, even when no external force is present, can produce unexpected results, as *face-stepping*. We discuss such phenomena using the so-called ξ -vector formulation and present known results from the mathematical point of view.

STANCU, Alina (Courant Institute of Mathematical Sciences, USA)

On evolutions of planar interfaces with crystalline energies

Motion determined by a crystalline energy is viewed as a typical example of geometric evolution by a nonsmooth boundary energy density. The evolution is specific to piecewise linear interfaces and is described by a system of ordinary differential equations for the support functions to the flat sides. These curves have no curvature in the conventional geometric sense (more precisely, the curvature is zero on each face and infinite at each vertex), but, following M. Gurtin and J. Taylor, one can still define a weighted curvature taking the first variation of the boundary energy within a restricted class of polygonal curves. As a result, the crystalline curvature is used to define an analogous motion by curvature and an evolution by surface diffusion for piecewise linear interfaces. In either case, up to some extent, there are different proposed models. We will discuss some of their properties from the point of view of having a unified theory, as well as their consistency with the corresponding evolutions for a smooth interface.

TAYLOR, Jean E (Rutgers University, USA)

Overview

The following issues in interface motion modelling will be surveyed: Diffuse versus sharp interfaces, differentiable versus non-differentiable surface free energies, variational versus PDE versus (systems of) ODE approaches. Particular attention will be paid to modelling triple junction energies and motion.



BIALECKI, Bernard (Colorado School of Mines, USA)

An orthogonal spline collocation alternating-direction implicit method for nonlinear parabolic problems on rectangular polygons

We consider a nonlinear parabolic initial-boundary value problem on a rectangular polygon with the solution satisfying variable coefficient Robin's boundary conditions. An approximation to the solution at the desired time value is obtained using an alternating-direction implicit extrapolated Crank-Nicolson scheme in which orthogonal spline collocation with piecewise polynomials of an arbitrary degree ≥ 3 is used for spatial discretization. For rectangular and L shaped regions, we describe an efficient B -spline implementation of the scheme and present numerical results demonstrating the accuracy and convergence rates in various norms. For problems with homogeneous Dirichlet boundary conditions, we observe a superconvergence phenomenon when the initial condition is approximated using the Gauss interpolant rather than the quasi-interpolant suggested by Douglas and Dupont for parabolic equations in a single space variable. This is a joint work with Ryan I Fernandes, Department of Mathematics, St Xaviers College, India.

CHRISTARA, Christina (Department of Computer Science, University of Toronto, Canada)

High-performance spline collocation methods for elliptic PDEs

Optimal spline collocation methods for elliptic Boundary Value Problems have been relatively recently developed, offering an alternative to Galerkin finite element methods as well as to Hermite spline collocation methods. Fast solvers, though, for spline collocation equations are still in the making. A variety of solvers has been studied, including acceleration techniques with various preconditioners and domain decomposition, but the analysis has been carried out for a few only solvers and for restricted classes of PDE operators. In this talk, we focus on two classes of solvers for quadratic spline collocation equations: (a) Multigrid methods and (b) Fourier methods. These solvers are shown to be optimal in their (sequential) computational complexity, that is, they compute the solution in time proportional to the size of the problem. The parallel implementation of PDE solvers is discussed, their communication requirements on distributed memory machines classified, and their computational complexity studied.

KARAGEORGHIS, Andreas (Department of Mathematics and Statistics, University of Cyprus, Cyprus)

Modified nodal spline collocation methods for elliptic boundary value problems

In recent years, much attention has been devoted to the development of modified spline collocation methods for boundary value problems for both ordinary and partial differential equations. In this paper, we first give a summary of the results of the application of modified cubic spline collocation methods to second order two-point boundary value problems. We then apply these methods to certain separable elliptic boundary value problems on the unit square. It is shown that these can be solved very efficiently using matrix decomposition algorithms.

This is a joint work with G Fairweather.

KIM, Sangdong (Kyungpook Nat'l university, Taegu, Korea)

Preconditioning polynomial spline collocation method to elliptic equations

In this talk we study a preconditioning polynomial spline collocation method for a second order of uniformly elliptic boundary value problem by a finite element method. It is shown that the distribution of eigenvalues for the established preconditioning system are well bounded in terms of the number of unknowns for a fixed degree of polynomial spline. Some numerical evidences are also provided.

SUN, Weiwei (City University of Hong Kong, Hong Kong)

Fast algorithms for solving high-order spline collocation discrete systems

We present a complete eigenvalue analysis for arbitrary order C^1 tensor product spline collocation applied to the Poisson equation on a rectangular domain. Based on this analysis, we develop a class of fast algorithms for solving the discrete linear systems.

CHATTERJEE, Siddhartha (University of North Carolina at Chapel Hill, USA)

Tune: Mathematical models, transformations, and system support for memory-friendly programming

The performance of an application on modern machines is dependent on, and extremely sensitive to, its memory hierarchy behavior. Good performance therefore requires "memory-friendly programming": careful layout of data structures, and restructuring of code and/or data use patterns to improve locality. The sophisticated algorithms used in modern scientific computing demand restructuring techniques that require expertise in computer architecture, burden the application programmer with tedious machine-specific details unrelated to program correctness, and reduce the readability, maintainability, and portability of the restructured code. The TUNE project aims to improve our understanding of locality for a class of "hierarchical" problems. We will discuss various aspects of the problem: developing the relevant mathematical techniques for representing and manipulating locality; characterizing the relationship between program transformations and numerical accuracy; implementing interactive and automatic locality management tools; and proposing and evaluating innovative memory architectures for future-generation systems.

DOUGLAS, Craig C (University of Kentucky, USA)

Cache aware multigrid for parallel supercomputers

All RISC based computers attain high performance using memory hierarchies to make up for memory chips not keeping pace with the speedup of processors. Multigrid combines several standard sparse matrix techniques. We investigate when it makes sense to combine several of the multigrid components into one, using bitwise equivalent, block oriented algorithms. By re-using the data in cache several times, the savings in run time can be predicted and substantial. Structured grid cases are treated for parallel computers.

POTHEN, Alex (Old Dominion University and ICASE, NASA Langley Research Center, USA)

Enhancing the cache performance of irregular computations by reordering data accesses

We study the cache performance of the kernel of an unstructured mesh code from computational fluid dynamics using an "on-the-fly" cache simulation tool. We reorder the data accesses in this computation with the Cuthill-McKee, Sloan, Nested Dissection, and Peano-Hilbert (space-filling curve) reordering algorithms, and report how the cache performance is enhanced by these orderings. We look at the number of cache misses generated by each statement in the kernel to explain the reasons why the reordering algorithms improve cache performance. We conclude that the CM and Sloan reorderings improve spatial locality, while Nested Dissection improves temporal locality.

TOLEDO, Sivan (Tel-Aviv University, Israel)

Strategies for designing cache-friendly sparse-matrix codes

The talk will describe techniques for exploiting cache memories in sparse matrix computations. Exploiting caches is essential for achieving high performance on almost all computers.

I will focus on techniques for matrix-vector multiplication, an important computational kernel in many iterative linear solvers, and on techniques for sparse-matrix factorizations. The techniques exploit caches by reordering the matrices without increasing fill or work, by utilizing elimination trees to schedule the computation, and by performing simple kinds of memory accesses as efficiently as possible.

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HAGUE, Stephen J (Numerical Algorithms Group, Oxford, UK)

Building PSEs - "Let a hundred flowers bloom"?

In this presentation, we will look at further examples of efforts to build problem-solving environments, e.g. the European Union-funded STABLE project - seeking to combine statistics and visualisation. Some insights into the construction issues in building as "next generation" mathematical PSE will be offered. We will then address the question: are common PSE software architectures emerging or is each PSE construction exercise, by its problem-specific nature, essentially going to remain as "one of a hundred flowers that will bloom in its own way" - to mis-quote St, Francis of Assisi. Some of the current and emerging standards that do or might have bearing on future PSE construction will be referenced, and specifically mathematical issues will be addressed too, within the modern computing context of the information super highway, distributed computing, powerful desk-top systems etc. The standards to be mentioned will include: CORBA, DCOM, OpenGL, MPI, MathML, OpenMP, OpenMath, BasicMath, and others, including emerging proposals in the area of high performance computing using the increasingly popular Java language.

POOL, James C T (California Institute of Technology, Pasadena, USA)

The PSEware project: Progress, issues and prognosis

Scientific and engineering problems are increasingly attacked by geographically dispersed, multi-disciplinary teams utilizing heterogeneous computing systems ranging from desktop systems to the most powerful parallel system accessible to the team. The PSEware Project has explored the provision of a toolkit for such users to construct their own Problem Solving Environments (PSEs). Adopting an application driven approach, the project has developed the Soliton Explorer and CAT/LSA, a sparse linear system analyzer, as testbeds. The experience gained in these testbeds is now being applied to the Virtual Test Facility under development by Caltech's Center for Simulation of the Dynamic Response of Materials.

SHAW, Gareth J (Numerical Algorithms Group, UK)

Mathematical modelling in industry: Reports on the decision and Julius PSE projects

An important aspect of problem solving environments is the presentation layer through which the user interacts with the environment. NAG is involved in two European projects which seek to provide this functionality through IRIS Explorer (NAG's visualization and application building system). This approach provides the PSE with visual programming and scripting capabilities.

This talk will report on these two projects: DECISION (design optimization) and JULIUS (numerical simulation). It will emphasise the way in which IRIS Explorer is used in both cases to provide a visual programming front-end, and is integrated with relevant standards such as CORBA.

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CHAMBOLLE, Antonin (CEREMADE, Université de Paris-Dauphine, France)

Discrete approximations and numerical computations for the Mumford-Shah functional

We will present various approaches for minimizing the Mumford-Shah functional. This functional, initially designed for the image segmentation problem, offers also a possible approach for the study of fracture propagation in elastic materials. Its minimization is difficult, not only because of its non-convexity but also because of the presence of a term penalizing the total length (surface) of the discontinuity set of the unknown function. We will discuss both finite-differences and finite-elements approaches and show practical results.

This is a joint work with Blaise Bourdin, LPMTM, Université de Paris-Nord.

DZIUK, Gerhard (Institut für Angewandte Mathematik, Universität Freiburg, Germany)

Computation of curvature dependent free surface flows and phase transitions

The numerical simulation of semiconductor crystal growth is an essential tool for the design of an efficient industrial production process. Frequently, such a simulation requires the computation of a moving melting zone with a free capillary surface and a free solid/liquid interface. The mathematical model is a coupled system which consists of a heat equation and the Navier-Stokes equations in the melt with a Marangoni boundary condition. A Stefan condition models the phase transition. Adaptive finite element methods are used for the solution of such problems. A consistent discretization of curvature is essential. This is a joint work with E Bänsch, B Höhn, A Schmidt, K G Siebert.

FALCONE, Maurizio (Dipartimento di Matematica, Università di Roma "La Sapienza", Italy)

Semi-Lagrangian schemes for front propagation problems and applications

We present some recent results on the approximation of fronts using numerical methods of semi-lagrangian type. Those methods are used to compute viscosity solutions of Hamilton-Jacobi equations connected to the level-set formulation of several front propagation problems. In this talk we will address some theoretical issues, such as the convergence of high-order semi-lagrangian schemes, the treatment of obstacles in the propagation process, the implementation of several types of boundary conditions (Dirichlet, Neumann, state constraints) and the parallel version of semi-lagrangian schemes. We will also show numerical results of several experiments (in 2D and 3D) dealing with applications to combustion and image processing.

FIERRO, Francesca (Dipartimento di Matematica, Università di Milano, Italy)

Numerical approximation of mean curvature flow with a forcing term

Forced mean curvature flow is the motion of an interface Σ according to the evolution law $V = \kappa + g$. Here V denotes the velocity of Σ in its inner normal direction, κ is the sum of the principal curvatures, and g is a given forcing term. We study the approximation of this flow via a singularly perturbed double obstacle problem, which differs from the usual Allen-Cahn approximation because it is insensitive to the choice of the potential. We investigate smooth flows and evolutions past singularities. Under suitable assumptions we prove that the zero level sets of the solution to the double obstacle problem converge to the generalized motion by mean curvature with forcing term. Further interface error estimate are established. Finally we present some numerical results.

This work is partially done in collaboration with Roberta Goglione.

MAKRAKIS, George N (Institute of Applied and Computational Mathematics, FORTH-Hellas, Heraklion, Crete, Greece)

High-frequency computations near caustics and applications in underwater acoustics

It is well known that although the usual harmonic ansatz of geometrical optics fails near a caustic, uniform expansions can be found which remain valid in the neighborhood of the caustic, and reduce asymptotically to the usual geometric field far enough from it. Such expansions can be constructed by several methods which make essentially use of the symplectic structure of the phase space. In this paper we efficiently apply Maslov's method of canonical operators, in conjunction with Hamiltonian ray tracing for defining the topology of the caustics, to compute high-frequency scalar wavefields near smooth and cuspid caustics. Comparisons of the numerical computations of Maslov's integral with usual geometrical optics calculations in model problems arising in ocean acoustics show excellent accuracy.

MASNOU, Simon (CEREMADE, Université Paris-Dauphine, Paris, France)

Image singular interpolation

Object recognition, robotic vision, occluding noise removal or photograph design require the ability to perform disocclusion. We call disocclusion the recovery of hidden parts of objects in a digital image by interpolation from the vicinity of the occluded area. It will be shown how disocclusion can be performed by means of level lines, the boundaries of level sets, which offer a reliable, complete and contrast-invariant representation of the image, in contrast to edges. Level lines based disocclusion, which consists in the minimization of some energy depending on the level lines shape, yields a solution that may have strong discontinuities, which is not possible with PDE-based interpolation. Moreover, the proposed method is fully compatible with Kanizsa's theory of "amodal completion".

MERRIMAN, Barry (University of California at Los Angeles, USA)

Level set methods for modeling epitaxial growth of semiconductor devices

Molecular Beam Epitaxy is a method for growing thin film semiconductor devices. We have formulated an "island dynamics" model for epitaxial growth, based on laws of motion for the partial monolayer ("island") boundaries, coupled to diffusive transport of the deposited atoms. This provides a continuum description in the lateral surface directions, but atomic scale discreteness in the surface height, which is the regime of practical interest. Level set methods are employed for computations based on this model. In this talk, we will present the island dynamics model and comparisons with traditional kinetic Monte Carlo simulations of epitaxial growth. This is a joint work with Russel Caflisch, Susan Chen, Mark Gyure, Myungjoo Kang, Christian Ratsch, Dimitri Vvedensky.

RUUTH, Steven (UCLA, Department of Mathematics, USA)

A simple scheme for geometrical optics and related PDEs

To approximate the propagation of waves in the geometrical optics limit, a variety of methods have been proposed. Lagrangian methods can become quite complicated because cells must be adaptively added and deleted to achieve stable, accurate results. Standard Eulerian methods, however, are designed to treat merging fronts and thus do not allow waves to pass through one another.

To achieve an Eulerian formulation appropriate for wave propagation, J Steinhoff, M Fan and L Wang recently proposed Dynamic Surface Extension (DSE) Methods. In this talk, we discuss a new DSE-Scheme which uses first arrival times to extend the surface representation onto a uniform mesh. Methods for the reflection, refraction and the curvature-dependent motion of fronts are discussed. A simple method for propagating intensity values is also given.

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BERLYAND, Leonid (Department of Mathematics and Center for Materials Physics, Penn State University, USA)

Homogenization for superconducting thin films with large number of vortices

We present several recent results on homogenization for superconducting materials: (a) Homogenized description of an ideal superconductor reinforced by a large number of thin insulating rods. The main mathematical feature of this problem is the degree boundary condition due to the quantization. (b) Periodic arrays of large number of vortices have been observed in superconducting thin films (e.g. Nb and YBCO films), which are widely used for microwave applications. We present a mathematical model which provides a homogenized description for such films in terms of the effective anisotropy tensor and the effective vorticity. We shall also discuss unusual features (non invariance) of the homogenized limit for the wave functions (joint work with E Khruslov). (c) For the Ginzburg-Landau Model we provide examples, which demonstrate novel features of the homogenized limit (e.g. its dependence on the domain size) due to nonlinearity.

BLOWEY, James F (University of Durham, Department of Mathematical Sciences, UK)

Mathematical and numerical analysis of some models for phase separation of N -component alloys

This talk concentrates on the mathematical and numerical analyses of some models for phase separation of N -component alloys modelled by systems of Cahn-Hilliard equations. In particular we consider issues relating to models where the quench is not shallow (leading to a logarithmic or non-differentiable potential) or the mobility is not constant (namely concentration dependent or degenerate).

DREYER, Wolfgang (Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany)

Trends in modelling micromorphologies of solids, Part II: Statistical mechanics and molecular dynamics of tin/lead alloys

The phase field model of decomposition processes in two phase binary alloys relies on a mixture theory that takes strain- and higher concentration gradients into account. These appear as nonclassical contributions to the free energy and affects the resulting constitutive equations for the stress and the diffusion flux. Three mechanisms turn out as driving forces for the temporal development of morphology: Classical diffusion initiates the process of decomposition. Surface tension controls the number, steepness and orientation of the interfaces within the micro structure. Thermo-mechanical stresses will also change the microstructure. The resulting system of field equations for the fields of strain and concentration is of elliptic/parabolic type. On the micro scale these three mechanisms are intimately related to each other. This can at best be illustrated when the phenomenological phase field model is grounded on Newtonian mechanics of atoms of type A and B that form a crystal lattice. In particular, this point of view explains the meaning of surface tension and its affinity to the non convex part of the free energy and to the eigenstresses. Moreover, the number of material parameter of the phenomenological theory can be drastically reduced.

FOREST, Samuel (CNRS/Ecole Nationale Supérieure des Mines de Paris, Centre des Matériaux, France)

Modeling size effects in crystals

Classical homogenization techniques are not designed to predict the effect of the size of the constituents on the effective behaviour of heterogeneous materials. They usually take the volume fraction and, in some cases, the morphology of phase distribution into account. This shortcoming is related to the fact that, in crystals, the elastoviscoplastic behaviour of each constituent within the aggregate may be different from that observed on the constituent alone (say the single crystal). Cosserat single crystal plasticity is used in this work to describe the influence of grain size on the effective hardening behaviour of polycrystals. For that purpose, three-dimensional finite element calculations of periodic multi-crystalline aggregates of different grain sizes are provided. The approach is then applied to the case of two-phase single crystal superalloys for which the behaviour of phase γ as a matrix turns out to be strongly harder than the isolated phase.

MULLER, Wolfgang H (Department of Mechanical & Chemical Engineering, Heriot-Watt University, UK)

Trends in modelling micromorphologies of solids - a review (Part I)

A quantitative understanding of the microstructural development of high-tech materials in an engineering structure is crucial in order to guarantee functionality as well as their reliable use during operation. From a more general point of view a micro-structure is a "composite" system, prone to all the typical thermo-mechanical shortcomings of heterogeneous systems. Specific examples of such composite behavior are γ - γ' precipitation and directional growth in Ni-base superalloys, ripening of tetragonal phase in cubic Zirconia matrix, or coarsening in tin/lead solder alloys. A key problem of a "composite" are residual stresses which arise during manufacturing or during use. Physically speaking, they can be due to thermal mismatch and micro-structural changes or, from a manufacturing point of view, to the method of joining that was used. Over time such stresses will lead to the degradation and, eventually, to the failure of the whole structure. After a brief introduction into the subject this talk will focus on the interaction between experiments and mathematical methods which, together, allow to assess the reliability of composite structures. The aforementioned material systems will be used as case studies in this presentation to illustrate the potential and problems associated with continuum and phase field theories which are capable to predict morphological changes.

NIETHAMMER, Barbara (University of Bonn, Germany)

Mathematics of the Lifshitz-Slyozov-Wagner theory of Ostwald ripening

The classical theory of Lifshitz, Slyozov and Wagner (LSW) describes Coarsening of particles of second phase in a matrix by a mean field model for the particle size distribution function. This theory neglects direct interactions of particles and is therefore only strictly valid in the limit of infinite distance between the particles. Nevertheless the theory allows to make predictions about the selfsimilar behavior of the system for large times which are partly seen in experiments. In this talk we want to compare several mathematical results with the predictions of LSW. We will discuss a derivation of the LSW-model by homogenization of the underlying free boundary problem. This approach shows the crucial quantities which are involved if one compares the mean field model with experiments. Furthermore we present rigorous results on the long time behavior of solutions to the model. These establish a sensitive dependence on the initial distribution of the particles and thus in general do not confirm the predictions of the classical theory.

NOVICK-COHEN, Amy (Technion-IIT, Israel)

Simultaneous phase separation and ordering: Allen-Cahn/Cahn-Hilliard systems

Allen-Cahn/Cahn-Hilliard systems can be quite useful in the modeling of simultaneous phase separation and ordering in binary alloy systems. Though phenomenological derivations are possible, we review a derivation of the model (Cahn & N.C., 1994) which is based on a quasi-continuum limit of semi-discrete lattice dynamics. This approach naturally yields a connection between the Allen-Cahn and Cahn-Hilliard mobilities, and can be extended to allow for both degenerate and nondegenerate mobilities. General features of the model are outlined, and questions of existence, uniqueness and regularity are discussed in both the degenerate and nondegenerate mobility cases (Dal Passo, Giacomelli & N.C., 1998).

OLSCHEWSKI, Juergen (Bundesanstalt für Materialforschung und -prüfung, Germany)

The effect of morphology changes in nickel-based superalloys: An overview on experimental results and model considerations

Single-crystalline nickel-based superalloys have become increasingly important as blade materials in gas turbines because of their high creep resistance. They are two-phase high-temperature structural materials strengthened by precipitates of the L12-long-range ordered gamma-phase coherently embedded in the disordered f.c.c. gamma-matrix. The lattice misfit between the matrix phase and the precipitates has a great influence on the development of internal (eigen-) stresses and eigenstrains that cause under severe loading conditions (applied stress, high temperatures) characteristic morphology changes which affect the material behaviour. The experimentally well known directionally coarsening (rafting) process, i.e. the formation of plate-like structures from initially cuboidal precipitates is strongly influenced by the sign and size of the lattice misfit, the loading direction and the elastic stiffness ratio (contrast) of matrix and precipitate. For an advanced design of turbine engines it is crucial to understand and to predict the material response of these alloys under morphology changes. In this paper, an overview will be given on the material response of superalloys due to morphology changes, and from an engineering point of view, an overview on both analytical models and RVE finite element analyses used to simulate the influence of equilibrium morphologies on the material response.

VAN LEEUWEN, Yvonne (Laboratory of Materials Science, Delft University of Technology, The Netherlands)

Phase transformations in low carbon steel - numerical simulation and experimental validation

The mechanical properties of steel (Fe-C alloys with ranges of alloying elements) can be greatly influenced by governing the phase transformations that take place during cooling down after hot-rolling the material. For steels containing small amounts of carbon (typically 0.9 at. high temperature phase austenite (gamma) to ferrite (alpha)). It is during this phase transformation that the eventual microstructure is formed, and hence the properties of the material strongly depend on the exact characteristics of this transformation. The accurate modelling of the kinetics of this transformation enables an optimisation of the cooling process and with that a better control of the final properties of steel. In the literature the kinetics of the gamma/alpha phase transformation often is assumed to be governed by the carbon diffusion occurring due to the transformation. Since ferrite contains only a very small amount (0.09 at. austenite near the alpha/gamma interface enriches in carbon to such an extent that it hinders the formation of more ferrite. Further formation of ferrite occurs when carbon diffuses away from the interface. Therefore the diffusion of carbon into the austenite matrix is the rate controlling process for the transformation. To simulate the transformation process, a model is being developed, and implemented in FORTRAN, that describes the transformation by means of a Monte Carlo simulation along the interface combined with the diffusion of carbon described by the finite volume method. The energy state of the volume elements considered in the Monte Carlo simulation is determined by both the surface energy and the Gibbs free energy, the latter being a function of both temperature and composition of the phases on either side of the interface.

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BELLA, G (University of Rome, Italy)

Digital physics simulations of reactive flows

We describe the basic ideas behind the extension of the Lattice Gas Automata method to include chemical reactions in multicomponent fluid flows. Various techniques to guarantee exact conservation laws are discussed. An application to catalytic conversion is presented and commented on. This is a joint work with M Bernaschi, S Succi, H Chen, C Teixeira.

COSSU, Rossella (Istituto per le Applicazioni del Calcolo, CNR Roma, Italy)

Color spaces for vectorial data visualization in computational simulation

We will present visual procedures to represent and investigate vector fields, based on the perceptual, uniform or device color models. This technique has been utilized for the visualization of data generated by a multigrid semi-implicit finite difference method applied to the solution of two-dimensional shallow water equations for the simulation of water circulation in natural basins. The direction and magnitude of the vector are visualized using specific color maps, look-up tables in the color ring form; the proposed visualization assigns to each vector just color values and produces an image preserving the salient properties of vectors: magnitude and direction.

MANZI, Cristina (Center of Advanced Studies, Research and Development in Sardinia, Italy)

Three dimensional mesh generation for the simulation of blood flow in complex human vascular districts

The simulation of human cardiovascular system is one of the latest challenges of Computational Fluid Dynamics. It has several potential applications in medical training and research and cardiovascular surgery. It also presents several difficulties, one of which is the need of treating rather complex geometries whose definition has to be extracted from data coming from medical apparatus. In this work we present the activity related to mesh generation which has been accomplished at CRS4 within a larger project whose aim is to build a "virtual laboratory" for the modern emodynamicist and cardiovascular surgeon. Mesh generation starts from geometries already extracted from data provided by non invasive medical analyses like Computed Tomography (CT) or Magnetic Resonance Imaging (MRI), and described by means of a geometry modelling library (Shapes) which provides the capability to operate on such complex geometries. The user may associate different grid spacing to the topological features of the model. The generation then proceeds by discretising the curves, surfaces and volumes of the model. It may account for non-conforming grids and a mixed structured/unstructured mesh structure. The generation process will be explained in some details as well as the integration between the generator and the geometry modeller. Meshes obtained both on synthetic and on real geometries will be presented.

PAPARONE, Luigi (CIRA, The Italian Aerospace Research Center, Italy)

ZEN: An industrial flow solver for complex aeronautical applications

During the last decade the need of effective solvers for simulating complex flow fields has been a driving force for the research community. At CIRA a Three-dimensional Navier-Stokes solver (ZEN) that allows to simulate on multiblock structured grids complex flows has been developed and widely applied. Some guidelines, based on our experience, on how to develop and manage this type of solver will be given. The main focus is on the discussion of practical problems to be faced during typical aeronautical applications. To this scope some recent results will be shown. This is a joint work with M Amato and P Catalano.

PISTELLA, Francesca (Istituto per le Applicazioni del Calcolo-CNR, Rome, Italy)

A stable explicit scheme for the numerical integration of the Gross-Pitaevskii equation

The achievement of Bose-Einstein condensation in trapped gases of Rubidium, Sodium and Lithium has provided great impulse to the study of many-body quantum statistical effects in dilute fluids at very low temperature (nanoKelvin range). At the simplest level, the mathematical description of these phenomena is based on the Gross-Pitaevskii equation. In this talk we present preliminary numerical results based on a two-dimensional finite-difference scheme in cylindrical coordinates with explicit time marching. Numerical simulations aimed at assessing the stability/accuracy/efficiency of the numerical scheme will be presented and commented on. This is a joint work with M M Cerimele and S Succi.

SPITALERI, Rosa Maria (Istituto per le Applicazioni del Calcolo, Rome, Italy)

Linear and nonlinear multigrid computation for accelerated solutions

We present multigrid finite-difference approximation methods to solve differential problems arising in grid generation and fluid dynamics. We have developed:- nonlinear multigrid algorithms for the solution of elliptic grid generation systems,- a linear multigrid solver for the shallow water equations. Both sectors are of interest for industrial applications. We present recent results on multigrid computation applied to the solution of test and concrete problems, along with evaluation of multigrid acceleration.

BOISVERT, Ronald F (National Institute of Standards and Technology, USA)

Java for numerical computing

The rapid and widespread adoption of the Java language and environment for network-based computing has created a demand for reliable and reusable numerical software components to support a growing number of scientific applications now under development. In this talk I describe both positive and negative aspects of Java when considered as a language and environment for numerical computing. Benchmarks which illustrate current levels of performance of key numerical kernels on a variety of Java platforms will be presented. Finally, the status of community activities, such as the Java Grande Forum, which aim to improve the environment for numerical computing in Java will be described.

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CHATTERJEE, Siddhartha (Department of Computer Science, University of North Carolina, Chapel Hill, USA)

High performance numerics in Java: The importance of design

The programming and execution models of Java is sufficiently different from those of Fortran that source-to-source transcription of Fortran into Java may be insufficient to produce high-performance numerical code. Is it possible to reconcile high performance and the object model of Java? We show that the answer is "yes", if one is prepared to re-design the internal organization of the library. We draw on our experience of creating Java versions of LAPACK and Bailey's multi-precision MPFUN library. We also examine the performance gap between Java and Fortran/C++, identify their sources, and present design-level solutions to some of them.

FERNANDEZ, Victor (Sun Microsystems Inc, USA)

A Java visualization and steering interface for the sun scalable scientific subroutine library (Sun S3L)

We present a Java visualization and steering interface for Sun's Scalable Scientific Subroutine Library (Sun S3L). The objective is to provide runtime visualization and steering to a parallel program executing on a cluster of Symmetric Multiprocessor machines (SMP's). The interface distributes computation and analysis over a network, exploiting best each environment and providing seamless access to computational resources. The interface consists of a visualization API for the computational server and a Java front end or visualization server. The visualization API builds on top of S3L's parallel array infrastructure available to the user via the S3L's toolkit functions. The Java front end user interface is layered on top of Java's Abstract Window Toolkit (AWT), the Java3D visualization API, Java sockets and Java's Remote Method Invocation. Performance considerations are presented based on the results of some example applications.

MOREIRA, Jose E (IBM, Thomas J Watson Research Center, USA)

Achieving high performance in numerical computing with Java

Java provides a wealth of features that can have enormous impact on the design and development of library interfaces for scientific applications. The use of polymorphism and inheritance influence the way in which the interfaces (signature and classes) are defined in each numerical subject area. If these features are not exploited, then the library becomes a FORTRAN- or C-like library written in Java.

PETZOLD, Linda (Computational Science and Engineering University of California, Santa Barbara, USA)

The JMPL reconfigurable interface for CSE applications development

Interface design for mathematical software for complex and rapidly changing scientific and engineering applications can be problematic. A 'fixed' interface requires considerable effort to update after each minor revision of the underlying program. In this presentation we would like to demonstrate one possible solution to this problem. "JMPL" - Java Math Package Launcher - is a highly reconfigurable GUI interface which provides the user with in-line tools to simply and quickly adapt to revisions, capability for seamless transport of data between old and new versions, facility for machine-independent import and export of configurations, and the capacity to build higher level applications by driving multiple programs from the same interface. JMPL uses a highly configurable "bootstrapped" object structure to map the underlying application's control and data flow onto a corresponding GUI interface. This allows the interface to shrink and grow without internal programming changes. We will describe the use of JMPL for several large-scale scientific computing applications. This is a joint work with Andrew Strelzoff.

RANA, Omer F (Cardiff University, UK)

Performance issues in the use of Java for distributed scientific applications

Java has become a language of choice for applications executing in heterogeneous environments utilising distributed objects and multi-threading. To deal with large datasets scalable data mining approaches for efficient implementation of On-Line Analytical Processing (OLAP) algorithms are required. Conventional Java implementations do not directly provide support for data structures often encountered in data mining algorithms, and lack a *defacto* numerical precision on various platforms. We describe a distributed framework employing task and data parallelism, and implemented in high performance Java (HPJava). We identify issues of interest for data mining algorithms, and discuss possible solutions for overcoming limitations in the Java Virtual Machine. Our framework supports parallelism across workstation clusters, using the Message Passing Interface (MPI) as *middleware*. We show how such a framework may support components implementing different data mining algorithms, and linked to various databases via JDBC/ODBC bridges. We also provide guidelines for implementing parallel and distributed data mining on large datasets, and analyse a proof-of-concept data mining application based on a neural network analysis algorithm.

TREFETHEN, Anne E (The Numerical Algorithms Group, Wilkinson House, Oxford, UK)

The Java library interface

Java provides a wealth of features that can have enormous impact on the design and development of library interfaces for scientific applications. The use of polymorphism and inheritance influence the way in which the interfaces (signature and classes) are defined in each numerical subject area. If these features are not exploited, then the library becomes a FORTRAN- or C-like library written in Java. In this talk we will discuss the issues involved in designing interface definitions, which exploit polymorphism or/and inheritance for the development of a numerical library in Java. We show that the use of this interface definition does not necessarily influence the underlying algorithm but can provide a rich environment. We will draw on several numerical application areas as demonstration. This is a joint work with Mishi Derakhshan.

WEIDMANN, Matthias (Technical University Munich, Germany)

Pure Java computational fluid dynamics: Collaborative engineering with a real-world application

Modern scientific computing faces advanced requirements: Parallel computing in order to achieve high performance, engineer-application interaction at run-time through processing tools in order to shorten the production cycle, and enabling collaborative teamwork among the engineers working together on one specific problem in order to gain additional insight to problem solutions. This talk addresses the combination of these requirements in the case of a remote work environment. As unique work platform for the simulation computation, the processing tools and the secure teamwork collaboration serves the World Wide Web and the Java programming language.

BOTTA, Nicola (Potsdam Institute for Climate Impact Research, Germany)

Numerical methods for conservation laws in the low Mach regime

When computing unsteady flows at low and zero Mach (M) numbers one faces the following difficulties: as $M \rightarrow 0$ (i) pressure gradients vanish as M^2 , but they do affect the velocity field at the leading order; (ii) energy fluxes must satisfy an elliptic constraint; (iii) the number of time steps required by explicit methods grows as $1/M$. Because of these difficulties standard numerical methods exhibit a dramatical accuracy and efficiency breakdown at low Mach numbers and completely fail in the limit $M \rightarrow 0$. We present a semi-implicit second order extension of standard finite volume methods for compressible gas dynamics. The extension requires the solution of two elliptic equations per time step and yields numerical schemes in conservation form. It allows any such scheme to accurately and efficiently compute variable density $M \rightarrow 0$ flows. This is a joint work with R Klein and T Schneider.

MUNZ, C-D (Institut für Aero- und Gasdynamik, Stuttgart, Germany)

An asymptotics based solution method for weakly compressible fluid flow

In the low Mach number regime, the flow velocity and the speed of sound differ by orders of magnitude. Thus, physical effects might develop on different scales. Numerical simulation schemes should therefore efficiently and accurately deal with local small length scale flow structures, such as vortex formation and transport, with long wave length phenomena such as acoustic waves, and with nearly constant global effects, e.g. temperature rise from the walls. To get a more detailed insight into the behavior of a flow at low Mach numbers and about the coupling of the different scales, a multi-scale asymptotic analysis of the compressible Navier-Stokes equations has been carried out. A short summary of the results will be given. It will then be used to develop a numerical scheme. Different effects will be accounted for by multiple pressure variables describing separately the global, long wave, and small scale effects. The numerical method proposed is a semi-implicit predictor-corrector algorithm. In the predictor step, the asymptotic equations are used to guess the global and large scale effects. Here, the resolution of small scales is not necessary, therefore a rather coarse grid is used. The corrector step can be viewed as an incompressible solver with compressibility effects acting as source terms. The grid in this step has to be fine enough to resolve the small scale structures. The coarsening factor between the two meshes is $1/M$. This scheme can be viewed as a physically motivated multi-grid approach with only two grids and with different sets of equations solved on the two meshes. When the Mach number tends to zero, the method converges towards an incompressible projection method. Numerical results will be shown for Euler and Navier-Stokes simulations in both, the low Mach case and the incompressible limit.

VAN DER HEUL, Duncan Roy (Delft University of Technology and J M Burgers Centre, The Netherlands)

Numerical solution of a nonconvex hyperbolic system of conservation laws for inviscid flow with almost incompressible to supersonic regimes

In the course of handling a highly demanding application a number of measures have been developed to improve the temporal/spatial accuracy and robustness of an (semi) implicit segregated solution method, which is able to handle compressible flows with Mach numbers in the range of 0 to 30 of a medium with a highly nonlinear nonconvex equation of state in a very efficient manner. The method has been applied to model sheet cavitation on hydrofoils and on industrial high performance centrifugal pump impeller blades.

VIOZAT, Cécile A (CEA, France)

Numerical error versus modelling error for a natural convection problem

Natural convection problems are commonly solved either using the "low-Mach-number" model which is derived from the "compressible" model by assuming that the Mach number is low, or using the "Boussinesq" model which besides assumes a small temperature difference. These problems can also be solved by using directly the "compressible" model. We focus on the computation of the steady state solution of air confined in a square box with an horizontal temperature difference. We investigate cases where the modelling error, introduced by the utilization of a simpler model instead of the "compressible" one, becomes larger than the numerical error. This is a joint work with H Paillère.

GROTE, Marcus J (ETH Zürich, Switzerland)

Nonreflecting boundary conditions for electromagnetic and elastic waves

Time dependent scattering problems in unbounded media arise in many applications such as acoustics, electromagnetics, or elasticity. Numerical methods can handle complicated geometries, inhomogeneous media, and nonlinearity. However, they require an artificial boundary, which truncates the unbounded exterior domain. To eliminate spurious reflection from the artificial boundary, we have devised *exact nonreflecting boundary conditions* for the time dependent Maxwell equations and the elastic wave equation. These boundary conditions are local in time and involve only first derivatives of the solution. Therefore they are easily combined with finite difference or finite element methods. Numerical examples demonstrate the improvement in accuracy over standard methods.

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MSP-201

PETROPOULOS, Peter G (Department of Mathematical Sciences, New Jersey Institute of Technology, USA)

Reflectionless sponge layers for 3D electromagnetic waves: A review

I will review the approach of reflectionless wave absorbing layers for truncating computational domains in which the transient 3D Maxwell equations are solved numerically. Further, the performance and cost of implementation of the discrete absorbing layer will be compared to that of discrete high-order and exact absorbing boundary conditions. Numerical results, obtained with 2nd- and 4th-order finite difference schemes and with a pseudospectral scheme, will be shown to demonstrate the versatility of the absorbing layer. Also, a realistic numerical scattering problem will be used to compare, for a fixed error due to the absorbing boundary, the performance and computational cost of the absorbing layer against that needed by high-order local and exact ABCs in 2 and 3 dimensions for Maxwell's equations.

SOFRONOV, Ivan (Keldysh Institute of Applied Mathematics, Russian Academy of Sciences, Russia)

Artificial boundary conditions on the basis of exact solution to the linearized Euler equations

We will talk about numerical coupling of a linear far field with Euler or Navier-Stokes equations describing stationary three-dimensional aerodynamic flows. The goal is to find artificial boundary conditions that could provide an accurate solution even by using computational domains of a sufficiently small size. The far field is supposed to be modelled by the Euler equations linearized about a uniform subsonic flow at infinity. In our approach, we use an exact analytical representation of a such far field in terms of surface potentials, and a method for numerical solution of governing equations in the computational domain. We are going to discuss preliminary numerical results of calculating test flows past a wing. This is a joint work with D Kröner, Freiburg.

SPECOVIUS-NEUGEBAUER, Maria (University of Paderborn, Germany)

Artificial boundary conditions for elliptic problems in systems of channels

Many problems in mathematical physics lead to the investigation of partial differential equations in unbounded domains Ω , one example is the flow of a viscous fluid through a system of channels. One method to compute the solutions in the unbounded domain is to approximate them by solutions of appropriate boundary value problems on bounded subdomains Ω_R , which exhaust the domain Ω as $R \rightarrow \infty$. In this talk a method is presented how to derive optimal local boundary conditions for the approximating solutions together with asymptotically precise error estimates.

HINZ, Andreas M (Technical University Munich, Germany)

Radially symmetric Schrödinger operators

Since the famous example of von Neumann and Wigner, radially symmetric potentials have given rise to surprising phenomena in the spectral theory of Schrödinger operators. For instance, it has been shown that the higher-dimensional analogue of the Mathieu operator has an essential spectrum consisting of bands of absolutely continuous spectrum, separated by intervals of dense point spectrum. We will report on numerical investigations into the distribution of eigenvalues in these intervals and on the somewhat surprising discovery of the Welsh eigenvalue, a discrete eigenvalue in the two-dimensional case.

MARLETTA, Marco (University of Leicester, UK)

Non-selfadjoint ODE eigenproblems

In this talk I will describe work on numerical solution of non-selfadjoint ODE eigenproblems. I will address, among others, the following issues: (a) what is the best formulation of the system for a shooting approach, bearing in mind the need for reliability; (b) what numerical methods give, for a fixed accuracy, a cost which is independent of the spectral parameter. Examples will be given including almost-singular problems and Orr-Sommerfeld problems.

TRETTNER, Christiane (University of Regensburg, Germany)

Boundary eigenvalue problems of Orr-Sommerfeld type

In this talk a spectral analysis of nonclassical boundary eigenvalue problems for ordinary differential equations of the form $N(y) = \lambda P(y)$ (of the type of the Orr-Sommerfeld equation) is presented. Special attention is paid to the properties of the eigenfunctions and associated functions, e.g. completeness, minimality and basis properties.

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 MSP-203
 MSP-204

BONNANS, J Frédéric (INRIA-Rocquencourt, France)

Second order analysis of optimal control problems with second order state constraints

We give a theory of second order necessary or sufficient conditions for optimal control problems with second order state constraints. This is a joint work with H Zidani and A Shapiro.

GUILBAUD, Thérèse (INRIA, Domaine de Voluceau, Rocquencourt, France)

Logarithmic penalty and shooting methods

We aim at solving optimal control problems with punctual inequality constraints on the control by a logarithmic penalty method. We analyse the central trajectory, that is the solution set of logarithmic penalty problems associated to the optimal control problem. The penalty is directly adjoined to the criteria, so that the convergence is to be seen in infinite dimensional spaces. Our study lies on second order sufficient conditions for problems with linear differential equation or semilinear elliptic state equation. A numerical study is done over various problems, in the context of shooting methods.

MALANOWSKI, Kazimierz (Systems Research Insitute, Newelska 6, Warsaw, Poland)

Characterization of Lipschitz stability of solutions to parametric optimal control problems

Parametric optimal control problems (O_h) for nonlinear ODEs subject to inequality control constraints are considered. We assume that, for a reference value h_0 of the parameter, a solution exists, and we are looking for conditions under which, for all h from a neighborhood of h_0 , locally unique solutions and Lagrange multipliers of (O_h) exist and they are Lipschitz continuous functions of the parameter. It has been already known that a sufficient condition of this property is that the *constraint qualifications* (pointwise linear independence and controllability) as well as *coercivity* are satisfied with a certain *margin of freedom*. We show that this *sufficient* condition is also *necessary*, provided that the dependence of data on the parameter is sufficiently strong. This is joint work with A L Dontchev.

MAURER, Helmut (Westfälische Wilhelms-Universität Münster, Institut für Numerische Mathematik, Germany)

Second order sufficient conditions for optimal control problems with free final time

We derive second order sufficient optimality conditions (SSC) for optimal control problems with control-state constraints and *free* final time. Via a standard technique the control problem with *free* final time is transformed into one with *fixed* final time for which general SSC are available. The resulting SSC for control problems with free final time can be verified numerically via bounded solutions of associated Riccati equations. We check SSC for the classical Re-entry and Earth-Mars tranfer problem and discuss further examples from electrical engineering.

RAYMOND, Jean-Pierre (Lab. MIP, Universite Paul Sabatier, Toulouse, France)

Second order sufficient optimality conditions for nonlinear parabolic control problems with state constraints

Optimal control problems for semilinear parabolic equations with distributed and boundary controls are considered. Pointwise constraints on the control are given. On the state variable, both integral and pointwise constraints are analyzed. Sufficiency for local optimality is verified under different assumptions imposed on the dimension of the domain and the nature of state constraints. This is a joint work with F Troltsch.

ZIDANI, Housnaa (INRIA Rocquencourt, France)

Second order analysis of optimal control problems with partially polyhedric constraints

We discuss second order necessary or sufficient conditions for a class of optimal control problems with polyhedric control constraints and in the presence of state constraints satisfying some specific hypotheses. This is a joint work with F Bonnans.

BLOCH, Tony (University Of Michigan, Ann Arbor, USA)

Reduction of constrained and interconnected mechanical systems

In this talk I will discuss various mechanical systems and their analysis of reduction to lower dimensional models. In particular I will consider systems with both holonomic and nonholonomic constraints and coupled systems. The latter includes coupled finite-dimensional systems as well as coupled finite- and infinite-dimensional systems such as a rigid body connected to a rod or a string. I will discuss normal forms for the reduction of systems with constraints as well as the related problem of reduction by symmetry. I will also discuss the stability and control of such systems and the roles of asymptotic and nonlinear or Lyapunov stability. In addition I will describe the related problem of dissipation induced instability and instabilities induced by coupling of a finite system to an infinite one.

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 MSP-205
 MSP-206

DOWELL, Earl H (Duke University, Durham, USA)

Nonlinear dynamics of aeroelastic systems

This paper is an overview of a research program for nonlinear aeroelasticity of aircraft and rotorcraft in forward flight conducted at Duke University and supported by the Air Force Office of Scientific Research and the Army Research Office. Theoretical and experimental investigations of aircraft and rotor aeroelastic stability and nonlinear response are described. Flexible airfoil and rotor blade models with geometrical and freeplay structural nonlinearities and the ONERA stall aerodynamic model are considered. Analytical and numerical solutions of nonlinear mathematical models and experimental methods for flutter and forced response in a wind tunnel environment are discussed. Correlations between theoretical and experimental results are presented and some significant conclusions are drawn. It is hoped that this paper will help provide improved fundamental understanding of the nonlinear aeroelastic behavior of aircraft and rotorcraft.

HOLMES, Philip J (Princeton University, USA)

The proper orthogonal decomposition and dimension reduction

I will describe the proper orthogonal or Karhunen-Loève decomposition (POD) in the context of representing spatio-temporal fields in fluid and continuum mechanics in general. This method, which generates empirical basis functions from experimental or simulation data, is particularly appropriate when a few "coherent structures" or "nonlinear modes" dominate the field in terms of, for example, kinetic energy. Since the POD is optimal in the sense of capturing average energy, projections of the governing equations into relatively small sets of empirical eigenfunctions, along with appropriate modelling to account for neglected modes, can yield low-dimensional models which capture key features of the original infinite-dimensional system. I will review the mathematical foundations of POD, and describe some of the difficulties one encounters in practical applications to fluid flows on large or unbounded domains. The material is largely drawn from: P Holmes, J L Lumley and G Berkooz (1996) "Turbulence, Coherent Structures, Dynamical Systems and Symmetry", Cambridge University Press.

KIRBY, Michael (Colorado State University, Ft Collins, USA)

Dimensionality reduction via well-conditioned mappings

One of the best known methods for dimensionality reduction is the Karhunen-Loeve transform, or principal component analysis (proper orthogonal decomposition, singular value decomposition). This empirical linear transformation is appealing given it is based on solving an eigenvector problem which produces an optimal spanning subspace. Alternatively, empirical nonlinear transformations may be generated by, for example, computational neural networks or radial basis function expansions. These (adaptive) mappings may be determined by solving both smooth and combinatorial optimization problems. Such nonlinear mappings have the advantage that they may be used to efficiently model manifolds (as opposed to subspaces). This talk will present an application of Whitney's embedding theorem to the data reduction problem and will introduce a new reduction technique, motivated in part by a (constructive) proof of the theorem. In this setting we introduce the notion of a "good projection". We show that it is useful to optimize empirical projections with respects to their nonlinear inverses, i. e., these should be well-conditioned. One possibility is the computation of the singular vectors of the secants of the data. This may be improved upon using an adaptive algorithm. A method for constructing the nonlinear inverse of the projection and a discussion of its properties will also be presented. Finally, well-known methods of data reduction are compared with our approach within the context of Whitney's theorem.

NAMACHCHIVAYA, N Sri (University of Illinois & Urbana Champaign, Urbana, USA)

Dimension reduction in random dynamical systems

This paper examines an interesting and important theoretical problem in random dynamical systems - the low-dimensional approximation of stochastic dynamical systems for the prediction of its dynamical behavior. One of the classical methods of such approximation is the method of stochastic averaging which involves the convergence of a sequence $\{x^\varepsilon(t)\}$ of processes parameterized by ε to a limit process in some specific sense. It is important that the limit process $x^0(t)$ obtained by this procedure be much more tractable mathematically than the true physical process, and the parameter value ε , corresponding to the physical process, be small enough to yield a good approximation. The most widely used sense of the limit is that of weak convergence of measures. The underpinning of the classical averaging method is a separation of time scales so that the state variables of fast time scales can be averaged while the equations of the slow variables are approximated. In developing a stochastic averaging scheme it is assumed that the random perturbations are small and the unperturbed nonlinear system is integrable. Then under small perturbations, the quantities that are first integrals start to vary slowly and the averaging principle permits us to obtain the equations governing the evolution of these slow variables.

REGA, Guiseppe (Universit  di Roma La Sapienza, Italy)

Reduced models for complex dynamics of high-dimensional structural systems from experimental observations

The paper illustrates bifurcation mechanisms and complex attractors in the experimental analysis of monodimensional structural systems from the viewpoint of dynamics dimension. For flexible systems (like suspended cable/mass) undergoing highly coupled nonlinear responses, quasiperiodic responses, toroidal chaos, or chaos ensuing from tori breakdown, the interest is in identifying for each new dimension exhibited by the dynamics, a new experimental configuration variable responsible for bifurcation and ensuing steady dynamics. This is made in the paper for a number of transition regions from regular to nonregular responses. Using the delay embedding and the proper orthogonal decomposition procedures combinedly, it is shown how, though being the system potentially infinite-dimensional, its nonregular response is actually low-dimensional in most cases. Recognizing meaningful proper orthogonal modes allows to associate to each class of complex response, a class of reduced (and minimal) analytical models able to describe its nonlinear dynamics. Within the framework of a reduction procedure, these can specifically be built in each region of the control parameter space either by using the identified proper orthogonal modes, or - getting hints from the latter - by projecting the system infinite-dimensional dynamics on the known basis of corresponding linear modes. This is a joint work with R. Alaggio and F. Benedettini.

TITI, Edriss S (University of California, Irvine, USA)

Rigorous estimates for the number of degrees of freedom in dissipative systems and for the small scales in turbulent flows

In this talk we will present the concepts of determining modes, nodes, volume elements and determining finite elements for the Navier-Stokes equations, and other dissipative systems, and we will relate these concepts to the Takens' Embedding Theorem. Conceptually, the number of these determining modes, nodes and elements is comparable to the number of degrees of freedom in turbulent flows, in the case of Navier-Stokes equations. We will derive rigorous estimates on the number of these degrees of freedom in terms of the physical quantities, such as the Reynolds number and the rate of dissipation of energy. We will compare these rigorous estimates with those provided by the conventional theory of turbulence using heuristic physical arguments. We will also present rigorous estimates on the dimension of the global attractor for the three dimension Navier-Stokes Equations in terms of the above mentioned physical quantities.

WRIGGERS, Peter (Technische Hochschule Darmstadt, Darmstadt, Germany)

Reduction methods and integration schemes for geometrically exact shells and rods

To get dimensionally reduced formulations of 3d continua, shells and rods can be modelled as one or two dimensional manifolds, the points may undergo translations as well as independent rotations. Considering rods and shells respectively as one and two dimensional manifolds, the points of which can undergo translations as well as independent rotations, shell or rod theories can be achieved as dimensionally reduced formulations of three-dimensional continua. The finite element method reduces the problem to a finite dimensional one. The POD method can be employed to determine the active degrees of freedom in the finite element solution. In conjunction with the nonlinear, or the postprocessed, Galerkin method the influence of the passive modes can be taken into account. In long time integrations, for accurate dynamics, robust integrators must be used. The algorithms have to preserve certain mechanical properties of the system, like the momentum, the energy, or the symplectic structure. Examples are given to illustrate the approach in this ongoing research.

BLISCHKE, Wallace R (University of Southern California, Los Angeles, USA)

Cost analysis of warranties

The cost of a warranty on a product depends on the type of warranty offered and on the life distribution of the item warrantied. In this paper, brief descriptions of some of the many types of warranties offered on consumer goods and on commercial and government acquisitions are discussed. Cost models for a number of warranties (free-replacement, pro rata, combination, reliability improvement) are presented. The models involve renewal functions, partial expectations, and a number of other complex functions. Methods for optimization of warranty terms are analyzed. In most cases, numerical methods are required for solution.

MURTHY, D N P (University of Queensland, Australia)

Product warranty and mathematical modelling

The paper will give a brief introduction to product warranty and the framework needed to study the different warranty related topics. It will then discuss the mathematical modelling issues for the study of these topics. The paper will conclude with topics for future research.

FISCHER, Paul F (Argonne National Laboratory, Argonne IL, USA)

Robust high-order algorithms for unsteady flow applications

High-order discretizations yield excellent transport properties and are well suited to modern cache-based computer architectures which favor data reuse. However, they are frequently unstable in underresolved situations and consequently often lack the robustness required of complex flows. We examine several techniques to stabilize high-order discretizations used in unsteady flow simulations at high Reynolds numbers, including the weighted ENO schemes developed by the team of Shu, and bubble-stabilized spectral element methods developed by Canuto and co-workers. We compare the effectiveness of these approaches in a number of example problems, ranging from the one-dimensional Burgers equation to three-dimensional transitional flows.

GARBEY, Marc (Center for the Development of Parallel Scientific Computing, Univ-Lyon1, France)

A new algorithm for the parallel computation of Navier-Stokes and reaction-diffusion systems

We present some new adaptive coupling and time-marching schemes for the efficient metacomputation of systems of PDE's that can be used, for example, when two distant parallel computers are linked by a slow network. We consider an example from combustion in liquid that involves a NS code running on a Digital true cluster (DTC) in the Institut de Physique du Globe de Paris (IPGP-Paris) with a combustion code running on a DTC in the CDCSP-Lyon. We have obtained for our 2D test case an efficiency of about 80 percent, using a 10Mb/s connection between the two parallel computers.

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KAPER, Hans G (Argonne National Laboratory, USA)

Sound synthesis for scientific sonification

In this talk we describe a collaborative project between researchers in the Mathematics and Computer Science Division at Argonne National Laboratory and the Computer Music Project of the University of Illinois at Urbana-Champaign. The project focuses on scientific sonification – the use of sound for the exploration and analysis of complex data sets in scientific computing. We will discuss general principles of digital sound synthesis, describe DIASS (a Digital Instrument for Additive Sound Synthesis), and present the results of some preliminary experiments.

STEWART, D Scott (Department of Theoretical and Applied Mechanics, University of Illinois, USA)

Approximation of detonation dynamics by the compressible Euler equations with singular source terms

We consider how to approximate detonation flows with a finite length reaction zone and spatially distributed chemistry where the reaction zone and shock is replaced entirely by a single discontinuous front. We present a model and numerical algorithm called a Program Burn (PB) that captures end states that are consistent with those found from the theory of Detonation Shock Dynamics (the asymptotic theory for weak detonation shock curvature). We compare exact solutions of the reactive Euler equations in cylindrical geometry with our version of the PB model and show that excellent comparisons can be achieved.

TROMEUR DERVOU, Damien (Université Claude Bernard - Lyon I, France)

Domain decomposition with local Fourier basis methodology applied to the Navier-Stokes and reaction-diffusion systems

We present applications of so-called local Fourier bases to a domain-decomposition (DD) methodology in space; (see Israeli et al. for pioneering work for Helmholtz's problem). New difficulties arise in the application of this type of DD to the biharmonic streamfunction formulation of the incompressible Navier-Stokes (NS) equations with nonperiodic boundary conditions. We have obtained a high-order accurate and efficient parallel solver for this system and for systems of nonlinear reaction-diffusion equations that enables us to investigate different behavior of Frontal Polymerisation solutions using techniques that do not require an a priori knowledge of the structure of the front.

CHANG, Rosemary E (SGI, USA)

Visualization of models with freeform surfaces

The complexity of models that can be visualized or rendered in realtime depends on both the processing speed of the graphics system and the implemented algorithms. As the technology advances, visualization algorithms must be revisited and tailored to the new computing environment. Certain parts of the algorithm may speed up and new bottlenecks created. This talk will discuss the new challenges to visualization algorithms, in particular to the tessellation of freeform surface for subsequent rendering on a graphics workstation.

LANDMAN, Kerry A (University of Melbourne, Australia)

Mathematics - the invisible achiever

Behind most of the manufactured objects we use every day, there are design considerations and process control issues in production, as well as questions of how the goods should be distributed. Nearly 100 business and industry projects have benefited in the past 14 years from the concentrated application of mathematics and computing at the annual Australian problem-solving workshop, MISG (Mathematics-in-Industry Study Group). Some recent projects from the food industry will be discussed.

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VAN DE FLIERT, Barbera W (University of Twente, The Netherlands)

Evaporation and stress-driven diffusion: a generalised Stefan problem in paint

Industrial mathematics is a hot topic in the Netherlands. The question whether to do industrial mathematics at the university is to be answered in the light of scientific interest (and output), financial resources, attraction for students, and the profile of the department or university. I will discuss an example that is motivated by both scientific and practical interest, coming from the coating industry. The mathematical model, basically describing the evaporation of the solvent in liquid paint, is a generalised Stefan problem, analogous to studies in phase transition problems. This model has led to new research questions in the mathematical theory of the (one-phase) free boundary problem. The idea of stress driven diffusion originates from the polymer industry. In the paint application, stress build-up has been observed but a tool for measuring and validating the stress in time, during the drying process, has not been available. The model gives a first guideline for experiments; for the company this involves doing long term research.

WRIGHT, Margaret H (Bell Laboratories, Lucent Technologies, USA)

Better, bigger and beyond

Modeling and optimization are staples in industrial applications of mathematics, with an enviable record of helping to solve problems from every conceivable area. The high-tech business of Lucent Technologies provides a rich source of interesting questions that have been studied by researchers from Bell Labs and their business-unit colleagues. This talk will describe three problems from different contexts-wireless systems, protocol verification, and fiber design-and then analyze the paths to their solution via modeling and optimization, along with the common features that led to success.

BERTOZZI, Andrea (Duke University, Durham, USA)

Undercompressive shocks in driven film flow

Nonlinear hyperbolic conservation laws have solutions with propagating 'shocks' or discontinuities. Compressive shocks satisfy an 'entropy condition' in which characteristics enter the shock on each side. Undercompressive shocks violate this condition. We show that scalar laws with non-convex fluxes and fourth order diffusion have stable undercompressive fronts, yielding such unusual behavior as double shock structures from simple jump (Riemann) initial data. Thermal/gravity driven thin film flow is described by such equations and the signature of undercompressive fronts has been observed in recent experiments. Unlike compressive fronts, undercompressive film fronts are stable to fingering instabilities.

CERF, Corinne (Université Libre de Bruxelles, Belgium)

Detecting the chirality of knots and links, with application to chemistry

The topological chirality of a molecule implies its chemical chirality. This is important because a chemically chiral molecule exists as two forms, a left-handed form and a right-handed form, which may exhibit different behaviours. For a knotted or catenated molecule, it is thus very useful to determine whether the underlying knot or link is topologically chiral. We shall present an original method to detect the chirality of knots and links, based on a topological invariant called the nullification writhe [C. Cerf, J. Knot Theory Ramif. 6 (1997) 621]. It is a numerical invariant of alternating links, very simple to compute, yet as powerful as the Jones polynomial as far as chirality detection is concerned.

DE PILLIS, L G (Harvey Mudd College, Claremont, USA)

Modeling Cancer Tumor Growth with an Optimal Control Approach to Chemotherapy

In a cooperative effort with clinicians and research oncologists, we have been investigating mathematical models of cancer tumor growth and chemotherapy treatment. Currently, there are in existence an array of such mathematical models, each of which tends to focus on simulating one or two important elements of the multifaceted process of tumor growth and treatment. In an effort to better understand how these various aspects of growth and treatment interact with one another, we have created a new mathematical model of tumor growth which incorporates multiple important elements of the growth process and the effect of their mutual interactions. We make use of basic optimal control to search for chemotherapy treatment protocols which, in theory, are improvements to the standard protocols in use today.

This work is being carried out in an active collaboration with Prof. Ami Radunskaya of Pomona College and Dr. Charles Wiseman, head of the Mathematics of Medicine group in the Oncology Institute at St. Vincent's Hospital in Los Angeles. Preliminary results and future directions will be discussed.

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ZENG, Yanni (Department of Mathematics, University of Alabama at Birmingham, USA)
Gas flow in thermal nonequilibrium and hyperbolic systems with relaxation

We study gas flow in vibrational nonequilibrium. The model is a 4×4 nonlinear hyperbolic system with relaxation. Under physical assumptions, properties of thermodynamic variables relevant to stability are obtained, global existence for Cauchy problem with smooth and small data is established, and large time behavior is studied in pointwise sense. We formulate the fundamental solution in a systematic way for a general linear system with relaxation. The fundamental solution provides insights to the behavior of the nonlinear system, and is crucial to obtain our pointwise asymptotic picture. We also clarify the relation between subcharacteristic condition and a dissipative criterion originally proposed for hyperbolic-parabolic systems.

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BONA, Jerry (University of Texas at Austin, Texas, USA)
Initial-boundary-value problems for nonlinear wave equations

Nonlinear dispersive wave equations have been the object of study for several decades. Generally, these studies have concentrated on these equations posed as pure initial-value problems. However, in practical situations, it is often the case that non-trivial boundary conditions intrude naturally in modelling. It is the purpose of this report to review recent work on initial-boundary-value problems associated with Korteweg-de Vries-type equations and other models for the evolution of small-amplitude, long waves.

CHAMPNEYS, Alan R (University of Bristol, UK)
Solitary waves and fourth-order equations; An overview

This talk will review questions of existence, multiplicity and stability of solitary waves in non-integrable models described by the two-degree of freedom reversible Hamiltonian systems. Such models arise in many applications, e.g. for $\chi^{(2)}$ nonlinear optics and other coupled NLS systems, water waves, elastic buckling and continuum models of discrete lattices. The aim is to classify different properties of the homoclinic solutions to such equations based on the linearisation about a trivial equilibrium. For simplicity the discussion shall be tailored to the fourth-order equation $u'''' + bu'' - au + f(u, u', u'', u''') = 0$.

DOUGALIS, Vassilios A (Mathematics Department, University of Athens and Institute of Applied & Computational Mathematics, FORTH, Greece)
Numerical solution of Boussinesq systems

We consider various Boussinesq systems that describe two-way propagation of long waves of small amplitude in nonlinear dispersive media. We discuss the well-posedness of several initial- and boundary-value problems for such systems, which we then solve numerically by fully discrete Galerkin-finite element methods. We derive error estimates for the underlying numerical methods, and describe the outcome of numerical experiments that simulate two-way propagation of solutions of such systems, as well as the generation and interaction of solitary-wave solutions.

GROVES, Mark D (Dept of Math, Loughborough University, UK)
Hamiltonian spatial dynamics methods for two and three-dimensional steady water waves

We examine the *gravity-capillary steady water-wave problem* for a three-dimensional fluid of finite depth bounded above by a free surface. The fluid is uniformly translating in one horizontal direction x and periodic in the other horizontal direction z . Starting from a variational principle, we show that the hydrodynamic equations can be formulated as an infinite-dimensional Hamiltonian system in which $x - ct$ plays the role of the time-like variable. We are then able to give mathematically rigorous existence proofs for infinite families of two-dimensional multi-crested solitary waves (which have no z dependence and decay to zero for large $|x|$) and three-dimensional generalised solitary waves which consist of a three-dimensional motion which decays to a two-dimensional periodic wave for large $|x|$.

SHEN, Sam (University of Alberta, Canada)

Forced evolution equations, bifurcation, stability, and collision of uniform solitons

This talk discusses solutions of the forced Korteweg-de Vries equation, forced cubic nonlinear Schrodinger equation and forced sine-Gordon equation. A user-friendly C++ software was developed to solve these forced evolution equations. Its algorithm is based upon the semi-implicit spectral method and does not require artificial dispersion terms. Some conspicuous solution behavior of the forced systems will be shown, which does not occur in unforced systems, such as the generation and collision of uniform upstream advancing solitons in a channel flow of water over a bump. The stationary forced Korteweg-de Vries equation can have multiple solutions, whose stability will be demonstrated.

SMITH, Ronald (Loughborough University, UK)

Alternatives to the Kadomtsev Petviashvili equations for shallow water waves

Kadomtsev & Petviashvili (1970) suggested Hamiltonian model equations for almost uni-directional weakly nonlinear water waves. Unfortunately, the equations are only applicable to a restricted class of initial conditions. This presentation elaborates upon the derivation given by Craig & Groves (1994) of one-way Hamiltonian approximations to the water wave problem to derive generalisations and alternatives to the Kadomtsev Petviashvili equation. This is a joint work with Jerry L Bona.

SUN, Shu Ming (Virginia Polytechnic Institute and State University, Blacksburg, USA)

Periodic waves of finite amplitude in a two-fluid flow

This talk discusses two-dimensional periodic gravity waves in a two-fluid flow without any rigid boundaries. Each fluid is inviscid, incompressible and irrotational. The density ratio of the upper fluid to lower fluid is between zero and one. To obtain the existence of large amplitude waves, the governing equations are transformed into a single nonlinear integral equation and the corresponding integral operator is compact. By using a global bifurcation theorem, it is shown rigorously that there exist periodic interfacial waves of large amplitude until either the bifurcation parameter goes to infinity or the function of the wave profile and its derivative are not in classical Hölder spaces.

TOM, Michael M (Louisiana State University, Baton Rouge, USA)

A regularized long wave-KP equation

A slightly modified version of the regularized long wave-Kadomtsev-Petviashvili equation of the form $(u_t + u_x + u^p u_x - u_{xxt})_x + \epsilon(u_{yy} - u_{xxyy}) = 0$, where $\epsilon = \pm 1$, and $p \geq 1$ is an integer, which arises in the study of two-dimensional water waves is considered. It is shown that the initial-value problem for this model evolution equation is locally well-posed in a suitable function class regardless of the sign of ϵ . This solution defined locally in time is shown to be smoothly extendable to the entire time-axis if $p < 4$, $\epsilon = \pm 1$ and for $p \geq 4$ (even), $\epsilon = +1$. For $p \geq 4$ and $\epsilon = -1$ or $p > 4$ (odd), and $\epsilon = +1$, it is shown that certain initial data lead to a solution that blows up in finite time.

ZHANG, Bingyu (University of Cincinnati, USA)

Forced oscillation and its global stability

Propagation of shallow water waves along a channel generated by a wave maker at the one end can be modeled by the Benjamin-Bona-Mahoney equation posed on the quarter plane. A question arises naturally: does the wave generated by the wave maker become eventually a time periodic wave if the boundary forcing is periodic? The lab experiments and the numerical simulations conducted by Bona, Pritchards and Scott in 1980 indicate that with the presence of dissipation, if the amplitudes of the boundary forcing is small, then the solution of the equation becomes eventually time periodic. In this talk we will discuss how these lab and numerical simulation results can be demonstrated mathematically.

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CAGNOL, John (Ecole des Mines de Paris, France)

Shape control for hyperbolic problems via the second order shape derivative

In this talk we present the second order shape derivative for a class of hyperbolic problems. The first order derivative for those equations has been studied and relies, for non regular data, on the hidden regularity. Nevertheless the iteration to the second order is not straightforward: the data (especially the right-hand side) can no longer be the restriction to a domain of a function defined on an hold all. We need to consider the more general case where the functions are different on each domain, with a shape differentiability requirement. Moreover the boundary condition needs to be non homogeneous. A special emphasis is given for non regular boundary conditions which is important in the control theory framework. Our discussion will continue with the characterization of that second order shape derivative using the manifold derivative. This is a joint work with Jean-Paul Zolésio.

DELFOUR, Michel C (Centre de Recherches Mathématiques, Canada)

New intrinsic differential geometric methods in control and design: overview and examples

Over the past few years a new approach has been developed for the modelling and control of thin and asymptotic shells. The technique which is based on the extension by the projection of functions defined on the underlying submanifold to a neighbourhood in the ambient Euclidean space now rests on firm function analytic grounds including self-contained definitions of Sobolev spaces, trace theorems, regularity, etc. This bring sweeping simplifications in the analysis. Some examples are given to control and design problems as an illustration.

TRIGGIANI, Roberto (University of Virginia, USA)

Riemann geometric methods in control theory for partial differential equations

Riemann geometric methods are discussed in obtaining Carleman-type inequalities for partial differential equations of hyperbolic or Petrowski-type with variable coefficient-principal part and energy level lower order terms. These inequalities then yield continuous observability inequalities as well as uniform stabilization inequalities. The method yields checkable, sharp conditions. Non-trivial examples may be given.

ZOLÉSIO, Jean-Paul (Ecole des Mines de Paris and CNRS, France)

Intrinsic geometry and variational principle in the Euler equation

We review result on weak flow associated with non smooth fields and give applications for incompressible Euler equation and large deformation in elasticity from an Eulerian view point.

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BINDER, Andreas (MathConsult GmbH; Johannes Kepler University, Linz, Austria)

Mathematical modelling and numerical simulation of a process in ironmaking

The modelling and simulation of making iron has to deal with many phenomena, the most important ones being the flows of the different phases, chemical reactions and the thermal behavior. The Industrial Mathematics Institute and MathConsult work together with VOEST Alpine Industrienanlagenbau, one of the world-leading manufacturers of steel-mills, on a fairly large project treating certain aspects of ironmaking. We present the mathematical background of this project and our experiences with the partnership between a university institute, a mathematical software company and an industrial partner. This is a joint work with Andrea Schatz.

MAASS, Peter (University of Potsdam, Math. Department and WiSenT GmbH, Potsdam, Germany)

Mathematics for automated archiving systems, the art of character recognition

Reliable methods for converting printed texts into ASCII- or Word-documents are well established for clearly printed modern text fonts. These methods however fail when applied to diffuse images, old texts (e.g. 19th century 'Frakturschrift') or other distorted texts (e.g. scratched or dirty letters on containers/ licence plates). This problem can be treated by a variety of mathematical tools from image processing such as non-linear diffusion equations and wavelet techniques. Optimizing these methods have lead to a patented OCR-preprocessing, which is now widely used in automated archiving systems. We present the mathematical background as well as the main features of the ARTEX (archiving and text recognition) software. This is a joint work with Martin Boehm.

STARK, Hans-Georg (FH Schweinfurt and TecMath GmbH, Kaiserslautern, Germany)

Towards multimedia archives for broadcasting applications

In November 1995 the ESPRIT project EUROMEDIA was launched and coordinated by TECMATH, a company producing mathematical software. The project consortium includes five major European broadcasters, namely England's BBC, Austria's ORF, Germany's SWF and SDR and Sweden's SVT. The second major technology provider was Digital Equipment CEC Karlsruhe, Germany. During this project a multimedia archive including comfortable video indexing and retrieval methods was developed. It is intended to make the production process more easy by allowing for a simple and comfortable access to the individual partner's TV-archives. In this talk an overview about the project goals, the developed system and the project history is given. This is a joint work with Peter Thomas.

CHRISTIANSEN, Peter L (Department of Mathematical Modelling, Technical University of Denmark)

Self-focussing in discrete, disordered and noisy media

Self-focussing and mobility of coherent excitations in discrete, disordered and noisy media is investigated. Results obtained by direct numerical simulations are compared to analytical results obtained by the method of collective coordinates when applicable. This is a joint work with Yu B Gaididei, M Johansson, J Juul Rasmussen, V Mezentsev, K Oe Rasmussen, D Usero, D Henriksen and L Vazquez.

FIBICH, Gadi (Tel-Aviv University, Israel)

Damping effects in critical self-focusing

We analyze the effect of damping (absorption) on critical self-focusing. We identify a critical value δ_{th} for the damping parameter δ such that when $\delta > \delta_{th}$ damping arrests blowup and when $\delta \leq \delta_{th}$ the solution blows-up at the same asymptotic rate as the undamped NLS.

GAETA, Alexander L (School of Applied and Engineering Physics, Cornell University, USA)

Nonlinear propagation of ultrashort laser pulses in dispersive media

We present recent theoretical and experimental results on the self-focusing of femtosecond laser pulses in transparent dielectric media. As the pulse propagates through the material, dramatic changes occur to its temporal, spectral, and spatial properties. For peak input powers below the threshold for critical collapse, the experimentally observed dynamical behavior is in good agreement with the three-dimensional nonlinear Schrödinger model that includes the effects of self-steepening and space-time focusing. Above the threshold for critical collapse, it is necessary to include additional nonlinear processes including multi-photon absorption and plasma formation, and we describe our recent theoretical and experimental results in this regime.

ILAN, Boaz (School of Mathematics, Tel-Aviv University, Tel-Aviv, Israel)

Vectorial effects in self-focusing

We analyze vectorial effects in self-focusing in an isotropic Kerr medium. We derive a new perturbed nonlinear Schrödinger equation (NLS), which accounts for nonparaxial and vectorial effects. We apply Modulation Theory to the perturbed NLS and derive a reduced system of ODE's, which describes self-focusing in the presence of nonparaxial and vectorial effects. Analysis and numerical simulations of the reduced system and the perturbed NLS show that vectorial effects act in conjunction with nonparaxiality to arrest blowup. In addition, vectorial effects breakdown the radial symmetry of the beam, thus enhancing filamentation. This is a joint work with G Fibich.

LEVY, Doron (Department of Mathematics, UC Berkeley and LBNL, USA)

Self-focusing in the complex Ginzburg-Landau limit of the critical nonlinear Schrödinger equation

We analyze self-focusing and singularity formation in the complex Ginzburg-Landau equation (CGL), in a regime close to the critical nonlinear Schrödinger equation. Using modulation theory [Fibich and Papanicolaou, Phys. Lett. A 239:167-173, 1998], we derive a reduced system of ordinary differential equations that describes self-focusing in CGL. Analysis of the reduced system shows that in the physical regime of the parameters there is no blowup in CGL. Rather, the solution focuses once and then defocuses. The validity of the analysis is verified by comparison of numerical solutions of CGL with those of the reduced system. This is a joint work with G Fibich.

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MOLONEY, Jerome V (University of Arizona, USA)

Role of the critical collapse singularity in sustaining a novel femtosecond light guide

The critical collapse singularity of the 2D NLS equation is shown to play a prominent role in forming and sustaining a novel intense femtosecond light guide in air. We will discuss how normal group velocity dispersion and plasma generation serve to regularize the collapse and allow for recurrent collapse events. Extreme compression in space and time forces one to include higher order perturbation corrections and vectorial aspects. High power femtosecond laser pulses break up into a sea of interacting light filaments. This is joint work with Michal Mlejnek, Ewan Wright and Miroslav Kolesik.

SULEM, Pierre-Louis (CNRS, Observatoire de la Côte d'Azur, France)

Collapse of nonlinear Alfvén wave

Dispersive Alfvén wave trains propagating along an ambient magnetic field (of modulus B_0) in a magnetized plasma are circularly polarized and their envelope obeys a scalar nonlinear Schrödinger equation, with possible coupling to magnetosonic waves. According to the β of the plasma (square ratio of the sound and Alfvén velocities), convective or absolute modulational instabilities with respect to transverse perturbations can lead to Alfvén wave filamentation (transverse collapse) with possible formation of sharp magnetosonic fronts. In the weak dispersion limit, this collapse proceeds with a roughly circular polarization, up to a critical transverse scale l_{\perp} such that $\frac{l_{\perp}}{\lambda} \approx (\frac{l_d}{\lambda})^{-1/2} (\frac{\delta E}{B_0})^{-1}$ where l_d measures the characteristic dispersive length, λ the Alfvén wavelength and $\frac{\delta E}{B_0}$ its relative amplitude. The wave then ceases to be circularly polarized and its amplitude saturates. In this regime, the envelope dynamics is governed by a vector nonlinear Schrödinger equation with anisotropic diffraction. Small scales are still formed but the amplitude remains bounded, and instead of foci, very strong gradients develop on elongated structures. S. Champeaux, T. Passot and P.L. Sulem, *J. Plasma Phys.* **58**, 665-690 (1997); *Phys. Plasmas* **5**, 100-111 (1998); *Phys. Plasmas* **6**, 413-416 (1999).

WANG, Xiao-Ping (Department of Mathematics, Hong Kong University of Science & Technology, Hong Kong)

A moving mesh method and applications to self-focusing problems

Computing the blow up solutions of PDE's is difficult, especially in high dimensions. We will present a general moving mesh method that can handle multiple blow up solutions. Applications to nonlinear Schrödinger equations of various form will be given.

ALAM, Rafikul (Indian Institute of Technology Guwahati, India)

An acceleration in spectral approximation of integral operators

Consider the eigenvalue problem (EP): $T\phi = \lambda\phi$, $\phi \neq 0$, where T is an integral operator on an appropriate Banach space X . A standard approach to numerical solution of (EP) consists of two steps. The first step is to discretize T , denote the discrete operator by T_n and solve the eigenvalue problem $T_n\phi_n = \lambda_n\phi_n$, $\phi_n \neq 0$. Normally, T_n represents a coarse discretization of T and (λ_n, ϕ_n) provides a crude approximation of (λ, ϕ) . The second step consists of developing an efficient iterative procedure to successively refine (λ_n, ϕ_n) to achieve a desired accuracy. However, the performance of this classical approach is strongly influenced by the location of an eigenvalue in the spectrum. If an eigenvalue occurs in a dense part of the spectrum then the rate of convergence of this approach becomes very slow.

The main purpose of this paper is to describe an acceleration procedure which achieve arbitrarily high rates of convergence while keeping the computational cost at a minimum. We show that the new approach converges at the rate $\mathcal{O}(\|(T - T_n)^r T\|)$, where r is a positive integer chosen arbitrarily. Thus, if necessary, by choosing a large r an ill-conditioned eigenvalue problem can be solved very efficiently. An outline of our approach is as follows. First we choose a positive integer r and consider the product space X^r . Next, we lift the eigenvalue problem (EP) to the space X^r : $T\Phi = \lambda\Phi$, $0 \neq \Phi \in X^r$. Then we choose $T_n : X^r \rightarrow X^r$ such that $\|T - T_n\| = \|(T - T_n)^r T\|$ and solve the eigenvalue problem $T_n\Phi_n = \lambda_n\Phi_n$, $0 \neq \Phi_n \in X^r$. Finally, we develop an iterative procedure for refining (λ_n, Φ_n) . For illustration, we present numerical results by considering a compact integral operator.

This is joint work with B V Limaye.

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D'ALMEIDA, Filomena D (Faculdade de Engenharia da Universidade do Porto, Porto, Portugal)
Double iteration Newton like refinement for spectral elements of integral operators
 Eigenvalue problems for compact integral operators can be solved approximately by using two-level Newton methods. This technique has the advantage of giving approximate solutions with the accuracy corresponding to a fine discretization without solving any linear or eigenvalue problem for it: only small linear or eigenvalue systems, corresponding to a coarse discretization need to be solved. This fact is very important since matrices arising from integral operator approximations are usually fully dense. The refinement process is inspired by Newton's method and the linear problem involved at each iteration is solved by a nested iterative process. The fine discretization matrix is used only to perform matrix-vector multiplications. The numerical examples are done on an integral operator for which the eigenvalues and bases for the corresponding invariant subspaces are known exactly. This is joint work with Mario Ahues and Alain Largillier.

LIMAYE, Balmohan V (Indian Institute of Technology Bombay, India)
Improving accuracy of approximate eigenelements of integral operators
 In order to find an approximate solution of the eigenvalue problem for a compact integral operator, several kinds of discretizations are used in practice. More accurate approximate solutions can be obtained either by the technique of an iterative refinement of the computed solution or by considering an approximate polynomial eigenvalue problem of higher order. The latter technique is known as acceleration. A comparative study of these two techniques is made. Situations where neither only iterative refinement nor only acceleration is likely to give the desired results are described. In such cases, a combination of iterative refinement and acceleration may be employed. This is a joint work with Rafikul Alam.

BLAKE, John R (University of Birmingham, UK)
Acoustic cavitation, sonoluminescence and sonochemistry
 The non-spherical nature of the collapse of bubbles in many practical situations is of tremendous importance, having implications in, e.g., ultrasonic cleaning, tanning of leather, and underwater explosives. In particular the high speed liquid jet which threads through a bubble on collapse, for instance near a rigid boundary, is of considerable significance. An impressive photographic record of the liquid jet was obtained by Crum using a bubble situated in the vicinity of a platform oscillating vertically at a frequency of 60Hz. (See for example, Prosperetti, A. 1984 Bubble phenomena in sound fields: part 2. *Ultrasonics* **22**, 115-124; Suslick, K. S. 1989 The chemical effects of ultrasound. *Scientific American* **260**(2), 80-86.) Using the boundary integral method, calculations are performed which mimic the behaviour of this system to take advantage of the photographs of the phenomenon, and which aim to aid the understanding of this phenomenon.

KOHNEN, Gangolf (Institut fuer Verfahrenstechnik, FB IW, Halle, Germany)
Developments in calculating bubbly flows using the Euler/Lagrange approach
 This contribution is devoted to the latest advances of the calculation of bubbly flows using the Euler/Lagrange approach. It will be subdivided into a fundamental part including physical aspects as the assessment of the bubble equation of motion, the strong interaction between the liquid and gaseous phase, and the bubble - fluid turbulence modelling. Besides, essential computational/mathematical aspects will be taken into account. In this connection the problem of applying efficient algorithms searching a bubble during the tracking process will be addressed. Moreover, some remarks about parallelization of the Euler/Lagrange approach are included. In addition, the suitability of experimental data for validating numerical models is an important issue. Finally, numerical results will be presented for bubbly flows in bubble columns and suspension processes in stirred reactors.

MAGNAUDET, Jacques (Institut de Mecanique des Fluides de Toulouse, France)
Some aspects of the lift force on bubbles
 The shear-induced lift force is of major importance for predicting bubble motion in sheared flows. In this talk I shall review some recent developments, essentially analytical or numerical in nature, in our understanding of this force and on its prediction. I shall discuss the case of low- and high-Reynolds-number bubbles and show how the physical mechanisms governing the lift force in both limits are connected. Examples of bubble motion in vortical and turbulent flows will serve to illustrate the prominent role of this force in two-phase bubbly flows.

POPINET, Stephane (Universite Pierre et Marie Curie, France)

Coupling of radial and translational motion in small viscous bubbles

A small bubble in an ultrasonic field is subjected to various forces and instabilities. Its radial pulsation couples to translational motion, producing the so-called Bjerknes force. In some theories of single bubble sonoluminescence (SBSL) these effects play a major role in enhancing bubble deformation.

We perform both full Navier-Stokes simulation of the axisymmetric fluid mechanics, and an ODE model of the bubble motion.

We then discuss the net effect of these forces on a bubble in sonoluminescence conditions. The difficulty in explaining the observed bubble position, jitter and deformation using the effect of the Bjerknes force alone is pointed out. This is a joint work with Stephane Zaleski.

TRYGGVASON, Gretar (University of Michigan, USA)

Direct numerical simulations of many bubbles

Direct numerical simulations of flows containing many bubbles are discussed. The Navier-Stokes equations are solved by a finite difference/front tracking technique that allows the inclusion of fully deformable interfaces and surface tension, in addition to inertial and viscous effects. A parallel version of the method makes it possible to use large grids and resolve flows containing $O(100)$ bubbles. Studies of the motion of two- and three-dimensional finite Reynolds number buoyant bubbles in a periodic domain and drops in a channel are discussed. The simulations have shown, for example, that at moderate and high Reynolds numbers, freely evolving bubbles rise slower than regular arrays but at low Reynolds numbers the opposite is true. An examination of the mean structure of the array also shows an increase in the probability of finding horizontal pairs of bubbles as the Reynolds number increases. The methodology has also been extended to flows with phase changes and an example of a simulation of boiling flows will be shown.

ALTAS, Irfan (Charles Sturt University, Australia)

A high accuracy defect-correction multigrid method

The solution of large sets of equations is required when discrete methods are used to solve fluid flow and heat transfer problems. Although the cost of the solution is often a drawback when the number of equations in the set becomes large, higher order numerical methods can be employed in the discretization of differential equations to decrease the number of equations without losing accuracy. For example, using a fourth order difference scheme instead of a second order one would reduce the number of equations by approximately half while preserving the same accuracy. In this talk we propose a defect-correction form of the high order approximations for some differential equations by using multigrid techniques. We also derive a fourth order approximation to the boundary conditions to be consistent with the fourth order discretization of the underlying differential equations.

GUPTA, Murli M (The George Washington University, USA)

High accuracy multigrid solution of convection-diffusion equations

We describe a number of fourth-order, compact, finite difference schemes for solving the convection-diffusion equations in two- and three- dimensions. The convection- diffusion equations are discretized on a uniform grid, and multigrid techniques are utilized to obtain highly accurate solutions. A number of test problems are used to validate the results.

KOUATCHOU, Jules (Morgan State University, School of Engineering, USA)

Multigrid solution of 3D convection-diffusion equations: stability analysis of a high-order scheme

In (Jules Kouatchou, *Asymptotic stability of a 9-point multigrid algorithm for convection-diffusion equations*, ETNA, Vol. 6, p. 153-161, Dec. 1997) we combined a 9-point compact high-order finite difference approximation and the multigrid algorithm to solve the 2D convection-diffusion equation. We proved both analytically and numerically that the method is asymptotically stable. Using a 19-point high-order scheme as discretization operator on all grid levels of the multigrid solver, we apply the same technique and extend the proof to the 3D convection-diffusion equation. Numerical examples are provided to validate the analysis.

SPOTZ, William F (National Center for Atmospheric Research, USA)

High-order compact schemes for viscous flows

A general approach for developing high-order accurate, compact differencing schemes has been developed by utilizing the governing differential equation to approximate truncation error terms. For viscous problems, this results in a method which is not only fourth-order accurate and requires no special treatment near boundaries, but is non-oscillatory for any cell Peclet number. This talk will concentrate on recent extensions of high-order compact methodology, first in the area of no-slip boundary conditions for the stream function vorticity equations, and second for extensions to time-dependent problems.

ALVARADO, Fernando (University of Wisconsin-Madison, USA)

Estimating power market conditions from network observations

Deregulation of electric utilities has led to a new competitive regime for utilities. Along with this concept, we now face some new problems. In traditional systems, one of the main tasks was to infer the status of the system based on metered observations. A variety of estimation techniques were used, including weighted least squares and least absolute value estimates. More sophisticated estimators were developed that included the ability to determine system parameters along with system conditions by the simple device of including some of these parameters as additional degrees of freedom in the problem. In all cases, the observations were of physical quantities. In the evolving deregulated environment there are a host of new estimation needs. The most unique among these is the estimation of market parameters: the various costs of the participants, estimation of the degree of market power, estimation of the price elasticities of the participants, estimation of the volatilities of prices, and estimation of the correlations among prices, both temporal and spatial. This presentation will address some of these new estimation needs and illustrate methods and ideas to deal with them in an effective manner.

CLEMENTS, Kevin A (Worcester Polytechnic Institute, USA)

A state estimation framework for detecting rogue power transactions

Undisclosed bilateral transactions are power trades between power generators and users that are not announced to the independent operator of a deregulated electric network. Whether intentional or not, such transactions can adversely affect the transmission capacity and other important performance characteristics of the network. A promising approach to detecting and identifying these so-called rogue transactions combines a hypothesis testing framework with a problem formulation that resembles optimal power flow, a constrained optimization problem central to efficient power system operation. Some of the key modeling and computational ideas underlying this approach will be described.

ILIC, Marija D (Massachusetts Institute of Technology, USA)

Measures for comparing performance of regulated and deregulated electric power industries

In this talk we first provide a mathematical formulation of a single (operations and planning) objective for the regulated power industry. This performance can be interpreted as a dynamic efficiency measure of the industry as a whole and is used throughout the paper as a benchmark for comparison. It is emphasized that under uncertainties it becomes critical to relate the processes taking place in real time (operations) to the processes relevant for future investments. This point, although well-understood, has not been actively used for decision making in the regulated industry. We propose that it is impossible to analyze risks and opportunities without closely relating the processes of real time operations, planning pricing and investments. Next, the same objective is re-formulated using a dual programming formulation in which decision variables are prices. This formulation helps interpret main objectives of the power industry from an economic point of view. Finally, the dual programming formulation is used to pose the sub-problem of transmission operations, pricing and investments as a process of risk/opportunities management in the decentralized industry. Conditions are formalized under which solving this subproblem leads to near-optimal performance as measured in terms of the industry as a whole. Understanding these measures is essential for establishing regulatory structures capable of inducing near optimal performance under industry restructuring.

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ABABOU, Rachid (Institut de Mecanique des Fluides de Toulouse, France)

Dispersive transport in random porous media: Particles, fluxes, concentrations, and moment inverse problem

The authors present a general scheme for solving tracer transport problems in heterogeneous multidimensional velocity fields, as occurs in particular in the case of random porous media. The scheme can be decomposed into three steps : 1) Direct numerical simulation of tracer transport based on Lagrangian tracking of particles (concentration packets); 2) Calculation of a finite number of spatial and temporal moments of particles; and 3) Solution of an inverse problem on the moments to obtain the space-time distribution of concentration (and mass flux density). The whole approach is based on a probabilistic interpretation of concentration (and flux density) via particle positions (and mass weighted arrival times). The third step above is the solution of the "Moment Inverse Problem" (MIP). Several schemes for regularising and solving this problem are discussed and tested. The approach can be used for reconstructing (numerically) the local concentration and flux fields. It can also be adapted and used for analysing mean quantities and global effects, for instance, the longitudinal macro-dispersion of transversely averaged concentration in a stratified random flow with or without local diffusion. The effects of local or molecular diffusion are taken into account via random walks, or Wiener processes in continuous time. Current extensions of this work include a generalization of the probabilistic concentration-based MIP approach to mass flux density, which is related to the distribution of mass weighted arrival times. This is joint work with Ali Fadil.

BOURGEAT, Alain P (University of St Etienne, France)

Scaling up filtration laws in randomly heterogeneous porous media, by stochastic homogenization

The technique of stochastic homogenization is applied to three typical situations of filtration through porous media in order to give the scaled up models. In the first situation we consider two-phase flows through porous media with only the proper rock properties (permeability and porosity) being randomly distributed, under stationarity and ergodicity assumptions. In the second situation we use additional mixing conditions like "strong mixing conditions" (i.e. the correlation function is of polynomial type) or like "exponential mixing conditions" (i.e. the correlation function is of exponential type) to give estimates of the closeness of the scaled up solution to the initial one. The last problem is considering the scaling up of incompressible two-phase flow when all the rock filtration-related properties are randomly varying (including the saturation-dependant rock properties like Relative Permeability curves and Capillary Pressure curves). The stochastic two-scales convergence leads to the definition of new "global rock-filtration" curves which appear in the homogenized equations.

CAMPILLO, Fabien (INRIA/LATP, France)

Homogenization of random difference operators and calculation of effective coefficient

We are looking for the effective permeability of a high-contrasted porous media using a random walk method introduced by J F McCarthy. The two-dimensional/two-components medium has a random checkerboard structure: at each square of the grid is assigned independently a value of permeability, either δ ($0 < \delta \ll 1$) with probability p , or 1 with probability $1 - p$. We study the general theory of the homogenization of difference elliptic operators (i.e. discrete elliptic differential operators) with rapidly oscillating coefficients. We set up usual tools (G-convergence, Γ -convergence, compensated compactness, etc) in this context. We state the homogenization theorem in the random case. We focus on the difference operators corresponding to the generators of the random walks.

MICHEL, Julien (Unité de Mathématiques Pures et Appliquées, ENS Lyon, France)

Large deviations estimates in stochastic homogenization

It is well known that the homogenized coefficients in the context of stochastic homogenization may be computed thanks to the Ackoglu-Krengel subadditive ergodic theorem (see Dal Maso-Modica). In this talk we will focus on the asymptotics of this convergence in an exponential scale, exhibiting a large deviations property of subadditive processes. We will also show some numerical examples of this convergence by means of a finite volume scheme, as well as the approximate computation of the action in the large deviation principle, in the case of the random chessboard for an elliptic equation.

This is a joint work with Laurent Piccinini, Université de Montpellier II, France and Marie-Hélène Vignal, Université Paul Sabatier Toulouse 3, France.

PIATNITSKI, Andrey (P N Lebedev Physical Institute, Russian Academy of Sciences, Russia)

Averaging of random nonstationary convection-diffusion equations

The averaging problem for parabolic equation $u_t^\varepsilon = \operatorname{div}(a(x/\varepsilon, t/\varepsilon^\alpha)\nabla u^\varepsilon) + \varepsilon^{-1}b(x/\varepsilon, t/\varepsilon^\alpha) \cdot \nabla u^\varepsilon$ with periodic rapidly oscillating coefficients, is studied; here ε is a small positive parameter, $\alpha > 0$. It is shown that the limit behaviour of solutions depends crucially on whether $\alpha \geq 2$ or $\alpha < 2$. In the former case after introducing appropriate moving coordinates, we obtain a diffusive limit behaviour of the solutions, i.e. for some constant vector β the family $u^\varepsilon(x - \beta t/\varepsilon, t)$ converges to a solution of a parabolic equation with constant coefficients. For $\alpha < 2$ more complicated change of variables is used, it involves rapidly oscillating in time functions. In the case of random dynamics (in other words, in the case when the coefficients are random in time and still periodic in spacial variables) the solution u^ε converges in law to a solution of a suitable martingale problem.

ASLAM, Tariq D (Los Alamos National Laboratory, USA)

Level set algorithms for tracking discontinuities in hyperbolic conservation laws

A level set algorithm for tracking discontinuities in hyperbolic conservation laws is presented. The algorithm uses a simple finite difference approach, analogous to the method of lines ENO scheme presented in C-W Shu and S Osher, *Efficient Implementation of Essentially Non-oscillatory Shock-Capturing Schemes*, Journal of Computational Physics, **77**, 439-471, (1988). The zero of a level set function is used to specify the location of the discontinuity. Also, two solution states are used at all computational nodes, one corresponding to the "real" state, and one corresponding to a "ghost node" state, analogous to the "Ghost Fluid Method" of RP Fedkiw, T Aslam, B Merriman and S Osher, *A Non-Oscillatory Eulerian Approach to Interfaces in Multimaterial Flows (The Ghost Fluid Method)*, submitted Journal of Computational Physics, (1998). The resulting schemes are accurate, robust and easy to implement.

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KARLSEN, Kenneth H (Department of Mathematics, University of Bergen, Norway)

A fast level set method for reservoir simulation

We present a level set method for reservoir simulation based on a fractional flow formulation of two-phase, incompressible, immiscible flow in two or three space dimensions. The method uses a fast marching level set approach and is therefore considerably faster than conventional finite difference methods. The level set approach compares favourably with a front tracking method what regards speed and accuracy, but maintains the advantage of being able to handle changing topologies of the front structure.

LI, Xiaolin (SUNY at Stony Brook, USA)

Three dimensional front tracking and shock-contact interaction

In this presentation, we describe a simplified front tracking method for the simulation of fluid interface instabilities in high dimensions. This includes a simplified algorithm for the numerical description of interface geometry and the partially tracked algorithm for the shock-contact interaction in the study of multi-dimensional Richtmyer-Meshkov instability. These algorithms have greatly enhanced the capability of the Front Tracking method as an active tracking scheme and a direct interface propagation method.

RIDER, William J (Los Alamos National Laboratory, USA)

Stirred, but not shaken, mixing the stretched and torn

Modeling interfaces has been a focus of computational physics in recent years. The issues associated with simplistic aspects of interface tracking are vexing. For instance, the regularizations in interface tracking often manifest themselves as numerical surface tension. These effects are uncharacterized despite their ubiquitous presence in simulations. Of greater complexity is the interaction of interfaces with vorticity and the dynamics of mixing. We present our current results in each of these areas.

SHYUE, Keh-Ming (National Taiwan University, China)

A fluid-mixture type algorithm for compressible three-phase flows

We present a simple interface-capturing approach to a model of compressible three-phase (solid-liquid-gas) flow in more than one space dimension. We use the Euler equations of gas dynamics as a basic system, and consider problems with three different fluid components: condensed matter, liquid, and gas, separated by interfaces for the computations. The algorithm uses a Mie-Grüneisen type equation of state as a basis for the solid-liquid-gas coexistence cells, and has a model equations written in quasi-conservative to ensure the correct fluid mixing when approximating the equations numerically with interfaces. A conservative front-tracking method based on a wave-propagation formulation is employed to solve the proposed system. Several numerical numerical are presented that show the feasibility of the approach to practical problems. This includes some tests of a shock wave in bubbly liquids and solid-liquid suspensions.

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HARTMANN, Michael (Technical University of Braunschweig, Germany)

Runge-Kutta methods for the validated solution of ODEs

We present a method for deriving sharp error bounds for Runge-Kutta methods. It is based on the Peano kernel representation of linear functionals. Applications to popular explicit and implicit methods are given. It is shown, how the error bounds can be used for the validated solution of initial value problems. Theoretical as well as numerical comparisons with Taylor series methods are presented. This is a joint work with Knut Petras, Technical University of Braunschweig.

LOHNER, Rudolf (University of Karlsruhe, Germany)

Enclosure of solutions of ODEs: past, present, and future

Rigorous computational enclosure methods for ODEs started with R E Moore's work on interval arithmetic in the sixties. He computed bounds using Taylor expansions and interval arithmetic. Other authors followed this line or used intervals and differential inequalities. Slow progress was achieved until about twenty years later when a rather reliable method against the wrapping effect was found and implemented in a program called AWA. Since then several authors started work on different methods (implicit, Padé-like, Runge-Kutta). Also new methods against the wrapping effect are being developed. We will review this promising development and give an outlook on yet unsolved problems.

NEDIALKOV, Ned S (Department of Computer Science, University of Toronto, Toronto, Canada)

On stepsize control and stability in validated methods for IVPs for ODEs

We discuss three factors that can restrict the step length in validated methods for IVPs for ODEs: (1) the algorithm for validating existence and uniqueness of the solution, (2) accuracy, and (3) stability. We demonstrate with numerical experiments that a Taylor series method for validation allows larger stepsize than the constant enclosure method. We investigate the stability of interval Taylor series and interval Hermite-Obreschkoff methods. We show that the stability of an interval method is determined not only by the stability function of the underlying formula, as in standard methods for IVPs for ODEs, but also by the associated formula for the truncation error.

NEHER, Markus (Karlsruhe University, Germany)

On the use of geometric series to bound the local error of Taylor methods

Interval Taylor methods for the validated solution of odes often consist of two parts. First, a coarse enclosure of the solution is calculated. The coarse enclosure is then used in the second part of the algorithm to gain refined bounds of the local discretization errors. To compute the coarse enclosure usually a fixed point iteration is used, which can result in rather small step sizes in the integration of the ode. We present an alternative enclosure method that uses geometric series to bound the local discretization errors without the need of a coarse enclosure. It works for odes with a special structure, and for very large step sizes. Numerical examples and a comparison with other methods will be given.

RIHM, Robert (University of Karlsruhe, Germany)

Validated predictor-corrector methods

The most commonly used algorithms for enclosing solutions of ODEs are based on explicit Taylor series methods. We introduce some implicit enclosure methods which also use Taylor expansions. We derive a predictor-corrector algorithm by combining an explicit and an implicit method. Its computational costs do not exceed those of the involved explicit method significantly. For many problems, however, the corrector tightens the enclosures of the predictor considerably. We apply our methods to various classes of problems and show theoretical and numerical results.

CAIRNS, Andrew (Heriot-Watt University, UK)

Risk management for pension funds

This talk will consider stochastic models for defined benefit pension funds. We investigate risk as it appears to the fund sponsor and also to the members of a fund. We will show how dynamic stochastic control theory can be used to devise optimal asset allocation and contribution strategies.

DELBAEN, Freddy (ETH, Zurich, Switzerland)

Is VaR really measuring risk?

The Value at Risk is currently being used to measure risk. Although the definition of VaR changes from one place to another, it seems that the interpretation as a quantile is the most commonly used mathematical description. As is well known, quantiles have strange properties that might lead to unwanted side effects. Also it turns out that VaR cannot be used to define the risk based capital needed to calculate risk adjusted returns. The idea is to change the definition of VaR in such a way that newly defined risk measures have more suitable properties.

KEMP, Malcolm (Threadneedle Investment Managers, UK)

How effective is dynamic hedging of derivatives?

This paper analyses how well derivatives exposures can be hedged using dynamic hedging. It explores some practical and theoretical ways in which the characteristics of dynamic hedging can be improved, and the implications of imperfect hedging on the reserves that entities writing derivatives ought to hold. The impact of market jumps and unforecast changes in market volatility are considered by back-testing hedging strategies using market data.

ROWAN, John (Bank of Scotland, UK)

Practical considerations of risk management for senior executives

This presentation examines the concerns of senior executives who are ultimately responsible for the risk appetite of the organisation. These executives answer to investors and the market who have a perception of the risk the organisation represents irrespective of what sophisticated risk modelling may say. A number of illustrations from modelling traded market risk will be reviewed in addition to techniques currently employed for measuring risk in retail bank balance sheets. The impact of strategic decisions on the risk levels in retail balance sheets will be reviewed including the advice and analysis which a risk management team may provide.

CARSTENSEN, Carsten (University of Kiel, Germany)

Numerical Analysis of a non-convex variational problem in micromagnetics

Micromagnetic phenomena in rigid (ferro-)magnetic materials can be modelled by a minimisation problem (M) which involves anisotropic energy and a saturation condition that causes non-convexities. Typically, minimising sequences in (M) develop finer and finer oscillations and their weak limits do not attain the infimal energy. Solutions exist in a generalised sense and the observed microstructure can be described by Young measures. A relaxation by convexifying the energy density yields a weak form (RP) that resolves essential global informations. The numerical analysis of (RP) faces convex but degenerated energy functionals in a setting similar to mixed finite element formulations. The lowest order conform finite element schemes appear infeasible and nonconforming finite element methods are proposed. An a priori and a posteriori error analysis is presented for a penalised version of the side-restriction that the modulus of the magnetic field is bounded pointwise. Residual based adaptive algorithms are proposed and experimentally shown to be efficient.

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LUSKIN, Mitchell (University of Minnesota, USA)

Theory and computation for the microstructure at the interface between twinned layers of Martensite and a pure variant

In joint work with Bo Li, we have obtained results on the numerical simulation of a needle-like martensitic microstructure observed in biaxial loading experiments conducted by C. Chu and R. James on single crystals of the shape-memory alloy Cu-Al-Ni. We utilize a geometrically nonlinear continuum model and energy minimization to simulate the complex microstructure observed at the interface between twinned layers of two variants and a pure variant. Our simulations exhibit twinned layers that form branches and bend as they approach the interface with the pure variant. Similar branching and bending was observed by Chu and James in their experiments.

PLECHÁČ, Petr (University of Delaware, USA)

Numerical approximation of microstructure with scales

In certain models of phase transitions in solids or magnetostrictive materials or in optimal design of composite materials small scales may play significant role when describing phenomena like hysteresis etc. Numerical approximation of such problems is a difficult task as the direct discretization would compel us to use extremely fine meshes. A variational formulation which lead to minimizers that exhibit fine oscillations on finite though subgrid scales will be presented. Approaches based on combination of numerical homogenization and relaxation will be discussed. Available error control will be briefly demonstrated on some computational models of practical interest.

PROHL, Andreas (Christian-Albrechts-Universitaet Kiel, Germany)

On different finite element methods for computing crystalline microstructures

The minimization of nonconvex functionals naturally arises in material sciences where deformation gradients of certain alloys exhibit (laminated) microstructures. From a numerical point of view, classical conforming and non-conforming FEMs give minimizers with their quality being dependent on the mesh in a crucial way. The goal of the talk is to propose a new discontinuous FEM that gives improved results in terms of rates of convergence for quantities describing approximation of the microstructure. These results are illustrated by computational experiments. Secondly, an adaptive strategy based on this discontinuous FEM is discussed in order to further improve on the accuracy. This is a joint work with M Gobbert.

ESTEVEZ SCHWARZ, Diana (Humboldt-University of Berlin, Germany)

Consistent initialization of differential-algebraic equations in circuit simulation

The simulation of electric circuits by means of modified nodal analysis (MNA) leads to index-1 and index-2 differential-algebraic equations (DAEs). To treat DAEs numerically consistent initial values have to be calculated. The consistent initialization of the DAEs obtained with MNA can be realized taking advantage of the special structural properties of this equations. A graph-theoretical algorithm that analyzes this structural properties with regard to the consistent initialization and its use are going to be presented. Examples will be discussed.

FELDMANN, Uwe (Siemens AG München, Germany)

Industrial applications of the new algorithms

The methods described in the other presentations of this minisymposium were implemented into an industrial circuit simulation tool "Titan". This enabled the chance to test their functionality, robustness and efficiency on real industrial applications. We have mostly chosen integrated circuits in bipolar and in MOS technologies with a circuit size up to 10^4 transistors (equations). Some results are presented and are compared with conventional approaches, showing the progress achieved and indicating possible directions for further work.

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GÜNTHER, Michael (TU Darmstadt, Fachbereich Mathematik, Germany)

Numerical integration methods adapted for electric circuit simulation packages

Automatic generation and numerical integration of network equations are the core of industrial TCAD packages. These tools allow short design cycles of VLSI circuits, e.g. dynamic memories. In general, these circuits are charge sensitive. To yield physically correct results, most simulation packages use a charge-oriented version of modified nodal analysis. This modeling approach leads to a linear-implicit system of differential-algebraic equations, with charges as differential variables. However, the physical quantities the user is really interested in - node potentials and currents - appear only in algebraic form. We introduce a Rosenbrock-Wanner (ROW) method that offers step size prediction and error control based directly on node potentials and currents - in contrast to the standard BDF approach. Many packages - such as TITAN, the circuit simulator of Siemens AG - supply the Jacobian with every function evaluation at very low additional costs. It is about only 1.4 times more expensive to evaluate both right-hand side and Jacobian than right-hand side alone. BDF methods - the today's standard approach in analog simulation - use this information very efficiently. We introduce different approaches that modify ROW methods in order to use this information efficiently, too. Stability and stepsize control of the new methods will be discussed with benchmarks from circuit simulation. This is joint work with Markus Hoschek.

SCHWARZ, Angela (Technische Universität München, Germany)

Modeling and simulation of high-frequency quartz oscillators

Circuit simulation is a standard task of the computer-aided design of electronic circuits. The generation of the circuit equations leads to differential-algebraic equations (DAE). For the analysis of oscillatory circuits periodic solutions are of major interest. For highly oscillatory circuits (e.g. quartz oscillators) the common transient simulation fails due to the large computational effort. Direct methods have to be used. We present a model and the resulting DAE-system of a quartz oscillator. The periodic solution of this system is obtained by solving the associated boundary-value problem. This is done by a highly efficient and specialized new version of the multiple shooting method.

HODGES, Stewart (Financial Options Research Centre, University of Warwick, UK)

Derivatives valuation and hedging in incomplete markets

Realistic models of financial markets are now coming to recognise that (because of phenomena such as jumps, stochastic volatility and trading costs) markets are incomplete and exact replication of derivatives is impossible. In this setting, the calculation of a single value from one particular martingale measure is of doubtful meaning. An alternative, which is explored here, is to obtain upper and lower bounds. In some cases useful bounds (and robust hedging strategies) can be obtained from no-arbitrage considerations with very weak assumptions about the underlying stochastic processes. In other cases we need to bring in risk/reward considerations and make more specific assumptions about the stochastic processes involved in order to get good bounds.

MØLLER, Thomas (Laboratory of Actuarial Mathematics, University of Copenhagen, Denmark)

Hedging of payment streams in insurance

We consider an incomplete financial market consisting of two assets, a stock and a savings account, and extend (in the martingale case) the approach of risk-minimization to the situation where the hedger's liabilities are described by a general payment process. Our extension opens the possibility of hedging and controlling to some extent the risk inherent in insurance contracts generating payment streams that depend on pure insurance risk as well as financial risk. Examples include general unit-linked life insurance contracts driven by Markov jump processes and claim processes from non-life insurance where claim size distributions are affected by traded price indices.

SMITH, Andrew (Bacon & Woodrow, UK)

Incomplete markets and financial product pricing

Financial derivatives have traditionally been priced on the theory that risk can be managed by hedging. Insurance markets have traditionally worked very differently, managing risks instead by diversifying a large number of units. In practice, neither hedging nor diversification work perfectly. Furthermore, both forms of risk management take place within an institutional setting, which incurs further associated costs to the shareholder, such as taxation, agency effects and dealing spreads. Andrew Smith will present some practical methods to adjust for these imperfections, applied to the pricing of financial products.

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WILKIE, A D (Heriot-Watt University, UK)

Autoregressive stochastic models for investment variables or what goes up must come down

The conventional academic model for representing the movement of many investment variables is the random walk model or geometric brownian motion. However, this model does not reflect consistently the reality that companies make profits and pay dividends. The speaker has developed a comprehensive stochastic model for investment and economic variables suitable for simulation over long time periods (i.e. years rather than the hours or days horizon of investment managers). This includes autoregressive features, cointegration of related variables, and can easily accommodate conditional heteroscedasticity (ARCH), jumps and fat-tailed distributions. Some aspects can be reproduced by continuous (Ornstein-Uhlenbeck) processes, others not.

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BURR, Ulrich (Forschungszentrum Karlsruhe

Institut für Angewandte Thermo- und Fluidodynamik (IATF), Germany)

Turbulent transport of momentum and heat in magnetohydrodynamic rectangular duct flow with strong side wall jets

Magnetohydrodynamic rectangular duct flows are characterized by strong wall jets at the walls parallel to the magnetic field and a core region with uniform velocity distribution. An increase of the magnetic field strength causes higher shear in the jet and strong turbulent flow is promoted in the near wall regions. Simultaneously the increasing field stabilizes the core. An experimental study is presented where local turbulent flow quantities are measured by a traversable combined temperature-potential-difference probe. The simultaneous measurements of time dependent velocity and temperature signals facilitates the evaluation of Reynolds stresses and turbulent heat fluxes. From the probe measurements it is seen that the turbulence structure is formed by large scale two-dimensional vortices with their axis aligned in the direction of the magnetic field. An increase of the magnetic field results in an enhancement of turbulent transport that may considerably increase the heat removal from the side walls.

LEBOUCHER, Laurent (Centre for numerical modelling and process analysis, University of Greenwich, UK)

Numerical simulation of internal flows at high Hartman and Reynolds numbers

Numerical computation of internal magnetohydrodynamic flows at high Hartmann numbers is limited by the resolution of boundary layers. Even adaptive meshes can fail in resolving Hartmann layers which may be better treated with analytical boundary conditions. Instabilities of magnetohydrodynamic shear and boundary layers parallel to the magnetic field are probably best treated with explicit time-discretisation because of the numerical diffusion associated with implicit schemes. However explicit method are likely to be numerically unstable if the electromagnetic terms are not discretised properly. Simulations of unstable magnetohydrodynamic layers in duct flows with standard finite volumes and appropriate discretisation and boundary conditions will be presented.

MOLOKOV, Sergei (Coventry University, UK)

Asymptotic structure of parallel layers at high Hartmann and Reynolds number

Magnetohydrodynamic flows at high Hartmann number are characterised by the presence of distinct flow subregions. The most important of the subregions are the core, and the Hartmann and parallel layers. The latter are able to carry part of the volume flux by high velocity jets and thus are more likely to be affected by inertia than the other flow subregions. The asymptotic structure of these layers at high Reynolds number is discussed. Examples of numerical calculations of a steady, two-dimensional flow in a sudden expansion and a cavity with differentially heated walls in a uniform magnetic field are given.

MOREAU, Rene J (Lab MADYLAM, Grenoble, France)

Inertial and 3D effects in MHD boundary layers

MHD shear flows between insulating Hartmann walls exhibit a strong tendency to become two-dimensional. In such conditions a quasi-2D turbulence exists, fed by the instabilities due to the shear and suffers a weak dissipation (ohmic and viscous) within the Hartmann layers. So far, although many experiments have demonstrated that inertial effects must play an important role, the classical theory for both the Hartmann layer and the core flow ignores them. Besides, the persisting small three-dimensionality of the core flow remains unclear. This paper aims at modeling these quite general inertial and 3D effects and shows a first application to the particular case of the MATUR experiment (see a paper at mini-symposium MSP-140). The model is based on a perturbation technique using the two small parameters $1/Ha$ and $1/Re$. The leading term just coincides with the classical theory. The next order in $1/Ha$ allows to introduce inertia into the Hartmann layer theory, and the next order in $1/Re$ allows to model the 3D effects within the core. From among the consequences of this development, the emphasis will be put on both the prediction of the recirculation driven by Ekman pumping in the MATUR experiment (under moderate magnetic field) and the limitation to two-dimensionality even under high magnetic field.

THESS, Andre (Ilmenau University of Tech., Germany)

Natural convection in a liquid metal heated from above influenced by a magnetic field

In many industrial applications of metal processing, natural convection within the melt is a highly unwelcome phenomenon. For instance, during electron beam evaporation of liquid metals, vigorous convective motion drastically limits the thermodynamic efficiency of the process. For typical process parameters the convective heat losses amount for up to 70% of the energy input at the metal surface. In this context we study both experimentally and numerically natural convection in a layer of liquid metal heated from above. Moreover, we show how convective heat losses can be significantly reduced by applying an external magnetic field.

MOHR, Marcus (Universität Erlangen-Nürnberg, Germany)

Multigrid methods for inverse bioelectric field problems

Several diagnostic applications in electrocardiography lead to inverse problems. e.g. calculation of heart voltages from measurements on the torso results in solving potential equations with overdetermined boundary data (Neumann and Dirichlet type) on some part of the boundary and none on the rest. These inverse problems are ill-posed and the corresponding discrete systems badly conditioned, even after regularization. Thus conventional iterative solvers converge very slowly and are extremely compute intensive. We investigate the use of multigrid as forward solver in standard iterative processes, as well as the possibility to solve the inverse problem directly with a multigrid approach. Joint work with Professor Ulrich Rude.

SCHULZ, Volker H (Interdisciplinary Center for Scientific Computing, University of Heidelberg, Germany)

Simultaneous multigrid SQP methods for optimal control problems

The focus of this talk is on large optimization problems derived from optimal control problems in PDE. They are solved in a direct discretization approach by simultaneous SQP methods. At the core of these SQP type methods lie *Karush-Kuhn-Tucker (KKT)* systems. They can be considered special saddlepoint problems which, however, differ from the ones from Stokes or Navier-Stokes discretizations. Novel numerical multigrid approaches are presented to the numerical solution of such KKT systems. Theoretical as well as numerical results are presented for practical problems.

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TA'ASAN, Shlomo (Carnegie Mellon University, USA)

One shot multigrid methods for optimization problems

In this talk we review the main ideas of the multigrid one shot methods for optimization problems. An efficient multigrid algorithm is based on a good smoother and on an accurate coarse grid approximation. Of the two, the smoother seems to be the most critical one for most optimization problems, and we therefore devote most of this talk to that part. We focus on the Hessian and its symbol in relation to the construction of efficient smoothers. This includes analysis of the differential level as well as the discrete level. We classify problems according to the condition number of the discrete Hessian and assess the need for preconditioners for accelerating convergence. Finite dimensional as well as infinite dimensional design spaces will be discussed. Examples from fluid dynamics will be given.

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BAUER, Irene (Interdisciplinary Center for Scientific Computing, Germany)

Numerical methods for optimum experimental design in DAE systems

Chemical processes are frequently described by differential-algebraic equations with unknown parameters, that have to be estimated from experimental data. Optimum experimental design aims at minimizing the experimental costs for data evaluation and maximizing the statistical reliability of the estimated parameters. The mathematical formulation leads to an intricate nonlinear state-constrained optimal control problem in DAEs which we solve numerically using a direct approach. The talk describes an efficient structured SQP-method for the numerical solution of the resulting nonlinear equality and inequality constrained optimization problem with emphasis on the evaluation of the quadratic sub-problems. Industrial applications are given in the following talks.

This is a joint work with Hans Georg Bock, Stefan Körkel, and Johannes P. Schlöder.

ESTLER, Manfred (Degussa AG, Hanau-Wolfgang, Germany)

Optimal experimental design for the parameter identification of enzyme catalytic processes

For the evaluation of biocatalytic processes the determination of enzyme stability - expressed by total turnover number, TTN [mole of product / mole of catalyst], or half-life [hours] - is of great interest. By means of a kinetic model turnover number or half-life can be calculated. Since the identification of kinetic model parameter for enzymatic processes is a challenging task, it will be shown that application of the optimal experimental design technique is necessary for the design of appropriate experiments, which maximize the information content of the measurements with respect to the model parameters.

This is a joint work with Andreas Bommarius, Degussa AG, Germany; Ekaterina Kostina, Hans Georg Bock, Johannes P. Schlöder, Interdisciplinary Center for Scientific Computing (IWR), University of Heidelberg, Germany.

HAARIO, Heikki (University of Helsinki, Finland)

Global criteria for optimal design

Traditional criteria for optimal design of experiments - D-optimality, for instance - are based on linear theory. For nonlinear models they are applied by linearizing the model. We give examples where this approach does not properly work. As an alternative we propose the use of global type criteria. The performance of various versions of them is compared to that of the traditional ones. New adaptive MCMC methods are employed to analyse the confidence regions of the parameters.

KUD, Alexander (BASF Aktiengesellschaft, Germany)

Sequential experimental design in reaction kinetics

The topic of this lecture is the application of the methods of nonlinear optimum experimental design to a practical example from chemical reaction kinetics. Modelling the process results in a nonlinear differential algebraic system. The model contains process engineering components such as feeds and temperature control. In a sequential approach to optimum experimental design and parameter estimation involving methods and software tools developed at the IWR of the University of Heidelberg, an experimental design was computed whose measurement data after 2 experiments permitted estimation of all unknown system parameters with a standard deviation of less than 1 percent. By contrast, an experienced chemist working intuitively needed 15 experiments to achieve estimates of comparable quality. This is a joint work with I Bauer, S Körkel, A Kud, O Würz.

BORRELLI, Robert L (Harvey Mudd College, USA)

Using computers in the introductory ODE course

Curricular reform these days seems to be edging closer and closer to an interdisciplinary approach in which students take a more active role in their own course work. In mathematics departments this approach usually involves laboratory-based activities in which students play a hands-on role in converting "word problems" into mathematical models and "solving" them. This talk will explore the use of computers for modeling activities in the first course on differential equations along with a few examples.

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KAPILA, Ashwani K (Rensselaer Polytechnic Institute)

Web-based modules linking mathematics and applications

Under a program called Mathematics Across the Curriculum (MATC), sponsored by the National Science Foundation, web-based instructional materials are being developed at Rensselaer. These are typically in the form of modules, used by the students with guidance from the instructor, in a mathematics course, or in a course from science or engineering. Some modules on topics from multivariable calculus will be presented. The talk will describe the manner in which the material is used in the classroom, and the students' reaction to it.

NG, Bart S (Indiana Univ. Purdue University at Indianapolis, USA)

An experimental course on mathematical modeling of physical systems

In this talk, we describe a course, currently under development by Asok K. Sen et al. at IUPUI, in which students are introduced to the art of mathematical modeling through a number of real-time experiments. For each of these experiments, the students learn how to derive the governing differential equations, carry out a complete analysis of these equations, and perform computer simulations as needed. Students are expected to use mathematics and "physics" in a complementary fashion to obtain maximal information about the behavior of the system under consideration.

SCHLEINIGER, Gilberto F (University of Delaware, USA)

An interactive module: Systems of ODEs with chemical engineering applications

An interactive, web-based instructional module will be presented that integrates teaching of systems of ordinary differential equations with Chemical Engineering applications. The module is designed to be used in class, with computers connected to a web server, and with an instructor present to guide students through its activities. This is part of a larger effort called Project Links.

SIEGEL, Michael (New Jersey Institute of Technology, USA)

The NJIT Capstone course in applied mathematics and statistics

In this talk, some of the experiences gained and lessons learned in the creation of a "laboratory" course in mathematics at NJIT will be discussed. The NJIT CAPSTONE course is intended to teach students to combine experimental and analytical methods, mathematical modeling, and numerical computation, and to apply these toward the study of real physical systems. The first semester of the course consists of case studies (modules) involving lectures, experimental demonstrations, and homework assignments. This is followed by a second semester involving faculty guided group research projects. The students write up their research, and present their work in a CAPSTONE seminar which is open to other students and faculty. Past case studies have included experiments and modeling of electronic rectifier circuits, free surface Hele-Shaw flow, and waveguides in optics. The goal of the CAPSTONE course is to significantly improve students' critical thinking, analysis and synthesis skills, and preparation to enter industrial research environments. The extent to which these goals have been achieved will be discussed.

FIELD, Martyn R (Hitachi Dublin Laboratory, Ireland)

Using a parallel factorised sparse approximate inverse preconditioner to solve large structural analysis problems

In this paper we describe the development of a new parallel preconditioner for the conjugate gradient algorithm. In the sequential case the most commonly used preconditioner is the incomplete Cholesky algorithm. This preconditioner cannot be effectively parallelised due to its inherently sequential nature. We have developed a preconditioner which directly approximates the inverse of the matrix and hence can be applied efficiently in parallel. We present results from using this preconditioner to solve a range of large structural analysis problems with up to 1.4 million degrees of freedom. We also demonstrate the scalability of this preconditioner on up to 128 processors.

LENHARDT, Ingrid (University of Karlsruhe, Institute for Applied Mathematics, Germany)

Parallel equation solving with preconditioned Krylov subspace and Schur complement methods

The application of Krylov subspace methods for parallel solution of linear systems of equations arising in nonlinear structural finite element analysis is presented. Using domain decomposition methods a partial stiffness matrix \mathbf{K}_i is computed on each processor. Parallel preconditioning is based on preconditioning of this partial stiffness matrices. Nonlinear computations with arc length methods require the solution of two linear systems with the same stiffness matrix. For ill-conditioned linear systems with multiple right hand sides direct methods usually are superior to the iterative ones, but they are hard to parallelize. For this class of problems a Schur complement method is presented and compared to local preconditioned iterative methods.

PADIY, Alexander (University of Nijmegen, Netherlands)

On a parallel multilevel solver for large-scale elasticity problems

An application of the additive multilevel iteration method to parallel solving of large-scale linear elasticity problems is considered. The results are derived in the framework of the hierarchical basis finite-element discretization defined on a tensor product $\hat{T}_{xyz}^{(i)} = \hat{T}_{xy}^{(i)} \otimes \hat{T}_z$ of one-dimensional grid \hat{T}_z and a sequence of nested triangulations $\hat{T}_{xy}^{(i)}$. The algorithm is tested on a number of model problems, arising from bridge foundation modeling. Parallel performance of the solver is reported for Cray T3E-600 (DEC Alpha 21164, 300 MHz, 3D-torus) and Sun ES/4000 (Sun UltraSparc-I, 167 MHz, shared memory/bus) computer systems.

SCHWEIZERHOF, Karl H (University of Karlsruhe, Germany)

On applications of parallel solution techniques for highly nonlinear problems involving static and dynamic buckling

For stability investigations of structural members in solid mechanics usually a static approach is preferred in combination with a finite element discretization. Such a procedure involves the computation of so-called stability points and mostly path-following algorithms in combination with eigenvalue analyses are needed to judge the postbuckling behaviour. For complex structures as silo shells the real problem is investigated including the time dependency of the buckling process performing a nonlinear transient analysis. Both type of analysis require a fine discretization thus parallelization of the complete solution is needed even with rather bad conditioning of the system matrices. Besides the adjustment of the time integration schemes for a fully parallel solution, it is also an important aspect to choose an efficient but still reliable preconditioning. The numerical applications show the advantages and limits of the various solution strategies in realistic industrial situations. This is a joint work with Th Rottner.

WIENERS, Christian (Institut für Computeranwendungen, Universität Stuttgart, Germany)

Parallel multigrid methods for Prandtl-Reuß plasticity

We present a parallel multigrid method for Prandtl-Reuß plasticity. The basis for the plasticity computations builds a flexible finite element library which supports adaptive multigrid methods for various discretizations. This is coupled by an abstract interface for the material evaluation at every Gauss-point. The equation in time is discretized by diagonally implicit Runge-Kutta methods. The algorithm is realized with the software package *UG*, which is fully supported in parallel. The performance is demonstrated by several examples in 2D with assumed plain strain and in 3D. We investigate the resulting displacements, stresses and hardening parameters after a complete loading cycle for different material laws.

ASLAN, Zafer (Beykent University, Turkey)

Modeling of environmental and climatic problems: prediction of wind and water erosion

Magnitude of wind and water erosion mainly depend on wind velocity, rain fall rate, slope and soil characteristics. The speaker will discuss the role of a small, meso and large-scale phenomena (local and synoptic fluctuations) on water and in erosion in countries like Turkey. The Fourier transform analysis for monthly average values of windy speed and rainfall rate has been considered, and amplitudes, phase angles have been calculated. This study presents some results on wind speed simulations and seasonal fluctuations of water deficit for the selected stations in different erosion risk and transition regions of Turkey. A strong large-scale influence is observed on water erosivity factor. Meso and small-scale fluctuations played important role on wind erosion in southern Anatolia in recent years.

KAPUR, Jagat N (Jawaharlal Nehru University, New Delhi, India)

A review of the teaching and research in developing countries

Industrial mathematics is an emerging area of science and technology. However, till recently due attention was not paid in the developing countries like India on the teaching and research of this field. Indian Society of Industrial and Applied Mathematics (ISIAM) was established in 1991 to take appropriate steps for the proper development of this field. The speaker will present his efforts as the precedent of ICIAM to develop this subject in Indian subcontinent.

MANCHANDA, Pammy (Gurunanak Deo University, Amritsar, India)

Current researches on financial derivatives in Afro-Asian countries

Award of 1997 Alfred Nobel Memorial Prize of Economics Sciences to Scholes and Merton has very well recognized the importance of mathematical methods in development of financial options and future contract on securities leading to new derivative exchanges around the world. These concepts are lucidly presented in their lectures at the award ceremony on Dec. 9, 1997, which are printed in the American Economic Review, June, 1998. As observed, to capture influence and interaction of time and uncertainly effectively requires sophisticated mathematical and computational tools. Recently the speaker, Kocvara, and Siddiqi have developed a fast algorithm for American options. In the first week of Oct. 1998 several speakers specially Karandikar, Karmeshu and Mahajan presented their current work on option pricing in a two days seminar in New Delhi organized by the Indian Academy of Sciences. A workshop in the last week of Feb. 1999 has been organized by the Indian Society of Industrial and Applied Mathematics at Hamdard University, Delhi where Schachermayer will present his work and interact with Indian workers of this field. A review of these researches will be presented.

SIDDIQI, Abul H (Department of Mathematical Sciences, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia)

Variational methods and image processing in the third world countries

Image processing is an important branch of Information Technology. In the recent past Fractal, Wavelet and Variational Methods have been extensively used to tackle problems related to image analysis specially image compression and segmentation. Updated references can be found in Morel, J and Solimini, S (Variational Methods in Image Compression, Birkhauser, Boston, 1995), Kovacevic, J and Daubechies (Proc. IEEE, Scanning Wavelets 84(1996) 507-687), Chambolle, A, Devre, R A, Lee, N Y and Lucier, B, (Nonlinear Wavelet image processing Variational problems, compression, and noise removal through wavelet shrinkage, Preprint, 1998) and Siddiqi, A H Ahmad, M K, and Mukheimer, A A (Current developments in Fractal image compression in Brokate, M. and Siddiqi, A H (eds). Functional Analysis and Current Applications in Science, Technology and Industry, Pitman Research Notes in Mathematics Series Vol. 377, Longman, London, UK 1998). The main object of this talk is to present a resume of researches carried out in this area particularly in the universities of India and Saudi Arabia with special attention to endeavors by M K Ahmad, A A, Mukheimer, P Manchanda, Faouzi, M Khene and S Khan.

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HEYMAN, Ehud (Tel Aviv University, Israel)

Exact and local solutions for pulsed beam propagation and scattering

The complex source pulsed beams (CSPB) provide wavelets for high resolution probing of the propagation environment. This problem is addressed here via a systematic procedure whereby complex space-time source coordinates are substituted into the spectral integral representations of the Green's functions in a particular environment, giving the response of that environment when the input is a PB. Closed form expressions for the response are then obtained by evaluating the integral via the spectral theory of transients (STT). Examples are provided for the interaction of a PB with a dielectric interface, with a metallic wedge, and with a smooth inhomogeneous medium.

KAISER, Gerald (Virginia Center for Signals and Waves, USA)

Realizability of acoustic and electromagnetic wavelets by real source distributions

Physical Wavelets, or Complex Source Pulsed Beams (CSPB), are exact, causal solutions of the wave and Maxwell equations obtained by extending the retarded Green function to complex space-time. Thus they represent, formally, the fields emitted by a point source with complex space-time coordinates. This is a very compact way of describing pulsed beams radiated by a circular aperture in REAL space whose center, radius, orientation, launch time, and pulse duration are determined by the assumed complex source coordinates. But it cannot be realized literally because it is impossible to place a point source at complex space-time coordinates. We will briefly review CSPB, then construct an equivalent source DISTRIBUTION in real space-time (no longer a single point) which yields the CSPB solution exactly. This source distribution is a generalized function concentrated on the physical aperture emitting the beam, and when the source coordinates become real, it contracts to the original point source giving the retarded Green function. We propose that it may be possible to realize CSPB in practice using such source distributions. This should be very useful, given the many ideal properties of such beams. This is joint work with Ehud Heyman, Tel Aviv University, Israel.

STEINBERG, Ben Zion (Tel Aviv University, Israel)

Local spectral expansions using pulsed beams

The complex source pulsed beams (CSPB) furnish a complete basis for local observable-based spectral synthesis of general transient fields. Their advantages over the more conventional plane waves or Green function representations stem from the inherent localization properties of the expansion and from the ability to track the propagators locally in the ambient environment. In this talk we review three expansion schemes for pulsed radiation and propagation: an angular spectrum of PB for pulsed point-source configurations, a PB summation in a full phase-space format for extended source configurations, based on the Windowed Radon (SST) Transform, and a biorthogonal set of PB for well-collimated source distributions. This is a joint work with Ehud Heyman, Tel Aviv University, Israel.

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MSP-246

BRAUNER, Claude-Michel (Mathématiques Appliquées de Bordeaux, Université Bordeaux I, France)

On the derivation of the Kuramoto-Sivashinsky equation

We prove instability of the travelling wave solution in a 2D free boundary problem modelling the propagation of near-equidiffusional premixed flames. Moreover the moving front is pointwise unstable. This model was used by Sivashinsky to derive the Kuramoto-Sivashinsky equation. We construct a solution which does not satisfy Sivashinsky's assumptions. For this purpose we transform the system in a fully nonlinear evolution problem which in turn can be viewed as a discrete dynamical system. This is a joint work with Alessandra Lunardi, Università di Parma, Italy.

DOLD, John W (UMIST, UK)

Flames with non-monotonic curvature-dependent propagation

Considering a flame to be a moving interface which propagates at a curvature-dependent speed, interesting features arise if speed is a non-monotonic function of curvature. Anti-diffusive instability appears in windows of curvature-space, and a connection with phase-separation, between different curvatures of the interface, can be made. In examining real combustible media that might exhibit this phenomenon, a mixed, slowly-varying and near-equidiffusional model for large activation energy is highly fruitful. It's study, asymptotically, provides a broad generalisation of more weakly nonlinear, lower-order models for flame-fronts, such as the Kuramoto-Sivashinsky equation in which propagation-speed only depends linearly on curvature. This is a joint work with A Shah.

GALAKTIONOV, Victor A (Department of Mathematical Sciences, University of Bath, UK)

Dynamical systems of inequalities with application to detonation problem

We show that given a nonlinear parabolic equation of reaction-diffusion type or a fully nonlinear one, it is possible to ascribe to such PDE a two, or in general four-dimensional dynamical system (DS) describing some evolution properties of the PDE. In fact, the evolution properties are described by the corresponding dynamical system of inequalities (DSIs). It is shown that for several models the DSIs defines an invariant set in the phase-space which gives some bounds on the solutions and their spatial derivatives. The corresponding estimates are applied to the fully nonlinear equation derive by Buckmaster and Ludford in 1986 and describing the instability of the famous Zel'dovich-von Neuman-Doering square wave of detonation in a duck. We prove that modified models with slightly different nonlinearities can describe a free-boundary propagation on the singularity level and derive the interface equation.

LEDERMAN, Claudia (Universidad de Buenos Aires, Argentina)

UNIQUENESS in a free boundary problem in deflagration flames

We consider the following free boundary problem: Find a function $u(x, t) \geq 0$ in $D \subset \mathbb{R}^N \times (0, T)$ such that $\Delta u + \sum a_i u_{x_i} - u_t = 0$ in $D \cap \{u > 0\}$, and $u = 0, |\nabla_x u| = \sqrt{2M}$ on $D \cap \partial\{u > 0\}$ ($M > 0$ constant). In addition, Dirichlet or Neumann data are specified on the parabolic boundary of D . This problem arises in combustion theory as a limit situation in the propagation of premixed flames (high activation energy limit). The problem admits classical solutions only for good data and for small times. Several generalized concepts of solution have been proposed, among them the concepts of limit solution and viscosity solution. We find conditions under which the three concepts agree and produce a unique solution. This is a joint work with J.L. Vazquez and N. Wolanski.

ROQUEJOFFRE, Jean-Michel (Laboratoire MIP, Université Paul Sabatier, Toulouse, France)

An asymptotic model for the propagation of flames with non-unit Lewis number

This talk will be devoted to the dynamics and numerical simulations of a spherical flame model with Lewis number < 1 . Asymptotics of the different regimes - propagation, extinction, convergence to a steady state - will be presented.

MITCHELL, Christopher J (Information Security Group, Royal Holloway, University of London, UK)

Mathematics of cryptanalysis - A brief introduction

This short talk is designed to provide the background cryptography necessary for the other two talks in the mini-symposium. The main types of cryptographic primitive in use are introduced (including ciphers, MACs, hash-functions, signature schemes, and key establishment schemes). The assumptions normally made when cryptanalysing a cryptographic primitive are presented, and the different types of attack relevant to the various classes of primitive are introduced.

MURPHY, Sean (Royal Holloway, University of London, UK)

Statistical techniques in cryptography

There are many problems in cryptography that are essentially statistical in nature. This talk will consider some of these problems and examine the ad hoc techniques that have been used to address them. These techniques are often examples of widely used statistical techniques such as the EM algorithm.

PRENEEL, Bart (Katholieke Universiteit Leuven, Dept. Electrical Eng.-ESAT/COSIC, Belgium)

Birthday attacks on cryptographic primitives

We consider conventional cryptographic primitives (block ciphers, stream ciphers, hash functions, and MAC algorithms) and discuss the progress in their design and analysis. It is shown that for almost all these algorithms the security level is only the square root of what one would expect. In some cases this square root (or birthday attack) is well known, but recently some new attacks of this type have been discovered. This talk presents an overview of these attacks and explains how birthday attacks can be prevented.

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MSP-248

KISELEV, Alexey B (Faculty of Mechanics and Mathematics, Moscow MV Lomonosov State University, Russia)

Hypervelocity collisions and orbital breakups mathematical modeling

The paper investigates the orbital breakups as a major source of space debris production. Different types of breakups under the influence of nonuniform internal loadings are regarded caused by internal explosions or hypervelocity collisions with debris particles. The worked out new thermodynamic criterion of destruction based on the critical value of energy dissipation in irreversible transformations makes it possible to determine the number and fluxes of fragments formed in breakups. The comparative analysis shows that distribution functions of the number of fragments versus mass have extrema strongly depending on peculiarities of breakup scenario that can produce essential difference from forecasts given by the accepted fragmentation models. Breakups caused by chemical explosions or hypervelocity particles impacting pressurized vessels different fluxes of fragments. This is a joint work with N N Smirnov and V F Nikitin.

NAZARENKO, Andrey I (Center for Program Studies of the Russian Space Agency, Russia)

The solution of applied problems using space debris analysis models

The model of the long-term evolution of the orbital debris evolution in low Earth orbits is presented. The basic principles of the model construction are discussed and the data on new yearly formed objects introduced in the model is described. The model enables to get the description of the current space environment containing particles larger than 0.1 cm and make the assessment of the probability of spacecrafts collisions with debris particles. The comparison of the results provided by the model with space debris measurements are discussed. Long-term forecasts of the space debris environment are presented.

POTTER, Andrew E (Lunar Planetary Institute, Houston, USA)

Orbital breaking events observations

The paper presents the results of observation and analysis of the long-term evolution of the fragments formed in orbital breakups of lost stages of rocket boosters. The cumulative fluxes of fragments determined in radar observations enabled to improve the breakup models. The observations shown the greater fraction of large fragments that testified the fact of nonuniform internal loading having been the reason for breakups. This is a joint work with P Anz-Meader.

SMIRNOV, Nickolay N (Moscow MV Lomonosov State University, Russia)

Mathematical model for space debris evolution, production and self-production

Space activity of the mankind generated a great amount of orbital debris, i.e. manmade objects and their fragments launched into Space, inactive at nowadays and not serving any useful purpose. Those objects sizing from hundreds of microns up to decimeters, traveling at orbital velocities, remaining in orbits for many years and numbering billions formed a new media named "space debris" and became a serious hazard to space flights. Thus this media wherein the space satellites operate nowadays should be taken into account, and its impact on the durability of space missions should be evaluated.

The paper presents the mathematical model for space debris evolution taking into account its production, self production in collisions and self cleaning of the Low Earth Orbits due to the influence of the atmosphere. The results of long-term forecasts of orbital debris evolution for different altitudes show that the chain process of debris self-production at different altitudes could take place at different times and bring to a total contamination of the orbit.

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MSP-250

KISELEV, Alexey B (Mech.&Math. Faculty of Moscow MV Lomonosov State Univ., Russia)

Computer simulation of density waves on the roads and computer simulation of density waves on the roads

The paper presents the results of numerical simulation of transport flows on the roads base on the continua model. The governing hyperbolic system of equations enables to investigate the density waves arising on the roads in unsteady regimes of transport flows. The paper presents the results of numerical simulation of transport flows on the roads base on the continua model. The governing hyperbolic system of equations enables to investigate the density waves arising on the roads in unsteady regimes of transport flows. This is a joint work with V F Nikitin.

SMIRNOV, Nickolay N (Mech.&Math. Faculty of Moscow MV Lomonosov State Univ., Russia)

Mathematical theory of traffic flows

The governing system of equations is derived describing the traffic flows. The characteristics of the system of equations make it possible to determine the velocity of weak disturbances in the traffic flows. Analysis shows that under certain conditions strong disturbances can arise in the flow with velocities exceeding that for weak disturbances. The model problems of traffic flows acceleration and slowing down are regarded. The optimal flux versus density diagram is determined and compared with experiments.

YUMASHEV, Michael V (Institute of Mechanics of Moscow MV Lomonosov State Univ., Russia)

Analytical method for transport flows characteristics development

Mathematical models describing transport flows incorporate usually a number of characteristic coefficients (model parameter). Those coefficients characterize the response of the system to variations of the road situation. The paper presents some analytical methods to develop the transport flows characteristic coefficients based on the averaged values of dynamic characteristics for a single vehicle.

FAOU, Erwan (IRMAR, Université de Rennes 1, France)

Complete asymptotic for linear elastic clamped elliptic shell

This lecture contains the description and recipe of the asymptotic development of the 3D displacement for a linear elastic clamped elliptic shell. Optimal error bounds are derived, related to the presence of boundary layer terms with different scales. Comparison between accuracies of different classical 2D shell models are made.

HAKULA, Harri (Helsinki University of Technology, Finland)

Resolving characteristic length scales in thin shells using high-order FEM

Depending on the loading, boundary conditions, and the shell geometry, the solution of a given thin shell problem can vary dramatically. Indeed, the solution of any shell problem is a linear combination of solution components corresponding to relevant characteristic length scales of the given setup. Currently the most robust solution strategy is to use high-order FEM with appropriate mesh design. Here, a set of benchmark problems for shells of revolution is presented. Every length scale deduced via asymptotic analysis is demonstrated including the very long range scales arising e.g. in certain configurations of joined cylinders.

MADUREIRA, Alexandre L (Pennstate University, USA)

Error estimates for hierarchical modeling

When dealing with elliptic equations in thin plate-like domains, one is tempted to take advantage of the geometry and, in a lower dimension region, pose an alternative problem that still captures the main features of the original one. Two pertinent questions are how to do this and how good will be the approximation. In this talk we will quickly review the hierarchical modeling approach, which consists of projecting the original solution into a semi-discrete space, in our case a space of functions with polynomial dependence in the transverse direction. Then we will show how to derive error estimates in various norms, as the thickness goes to zero or as the polynomial degree increases.

MARDARE, Cristinel (University of Paris VI, France)

New error estimates in the theory of elastic shells

In elasticity, the deformation of a shell subjected to applied forces is described by several models. While the three-dimensional model is derived directly from the classical principle of equilibrium in mechanics, the two-dimensional models are obtained by making some additional hypotheses, which are not justified by a physical law. We here justify some two-dimensional approximations of the three-dimensional model by establishing error estimates valid for any geometric configuration of the shell. This is a joint work with Veronique Lods.

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 MSP-251

MOTYGIN, Oleg (Inst of Mech Engrng Problems)

A suitable for computer realization method for boundary layer construction in the theory of thin plates

The general procedure of construction and orthogonalization of all polynomial solutions to an elliptic problem is adapted for the elasticity problem in a semi-infinite strip. The media is assumed to be anisotropic and is allowed to be non-homogeneous in the transversal direction. In the case when the strip is homogeneous, explicit formulae are obtained. For a laminated media the procedure is reduced to manipulations with matrices performed with the help of computer. Integral representations of the solutions in the general non-homogeneous media are presented. This is a joint work with Sergei Nazarov.

RÖSSLE, Andreas (Mathematical Institute A, University of Stuttgart, Germany)

Higher order responses of thin linearly elastic plates and their visualization

The limit behaviors of three-dimensional displacements in thin linearly elastic plates, as their thickness approaches zero is known for various lateral boundary conditions. In the generic case the leading term of the asymptotic expansion of the scaled displacement is a Kirchhoff-Love field. In this contribution, the situation is investigated when the generic leading term vanishes. Conditions under which the asymptotic expansion 'starts' later and the structure of the first non-vanishing term will be given for both hard clamped and free lateral boundary conditions. It turns out that there are essentially only three new cases uncoupling in membrane and bending. These higher order responses of the plate will be classified. Finally results of some numerical experiments will be presented, where the higher order responses are visualized. This is a joint work with Monique Dauge, IRMAR, Université de Rennes I, France.

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MSP-254

CAMPOS, L M B C (I S T - S M Aeroespacial, ISR, Lisboa, Portugal)

On sound scattering by sheared flows, including shear layers, boundary layers and duct modes

The acoustics of shear flows has several important applications in aeronautics, such as: (i) sound transmission to the interior of the fuselage of an aircraft through the boundary layer; (ii) sound propagation through the shear layer between two jets; (iii) duct modes in a nozzle with boundary layers near the walls. The simplest model is based on the acoustic wave equation in an unidirectional shear flow, which has been solved in the literature only in one case: a linear, homentropic shear flow. In this presentation are included exact solutions for four other shear velocity profiles: (i) an exponential boundary layer, representing the asymptotic suction profile; (ii) a shear layer with hyperbolic tangent velocity profile; (iii) a parallel-sided duct with a parabolic velocity profile; (iv) a linear homenergetic shear (non-homentropic). In all cases of supersonic jets can exist a critical layer, where the Doppler shifted frequency vanishes, and sound absorption by the mean flow can occur. The results presented include the acoustic fields (free and eigenvalues and eigenfunctions), scattering coefficients (for reflection, transmission and absorption) and energy considerations for several boundary conditions (e.g. rigid or impedance walls) and combinations of wave parameters and flow scales. Since the solutions are exact there is no restriction, for example, on the ratio of wavelength of sound to the scale of variation of the mean shear flow velocity.

MOHRING, Willi (Max-Planck-Institut für Dämmungsforschung Göttingen, Germany)

Energy conservation and reciprocity for sound propagation in layered flows

The relation between energy conservation and reciprocity between source and observer is studied for sound propagation in layered media. Unlimited regions with reflected and transmitted waves and regions bounded by a rigid or compliant wall with only a reflected wave and eventually a wall wave are considered. Energy conservation and reciprocity is discussed first for uniform flow and layered speed of sound where no ambiguity arises. Then flows with varying velocity are considered. These are rotational flows and several energy conservation laws have been proposed for this situation. The implications of these different laws on the reciprocity relation between sound and observer are described.

PIERCE, Allan D (ENG Aero & Mech Engineering, Boston University, USA)

The sound in and around a cavity due to grazing flow: a new method of calculation

A newly proposed *acoustic projection methods* used to develop the governing equations for the acoustic field in and around a two-dimensional cavity subject to grazing flow. The resulting governing equation is then solved computationally. The method has three distinguishing features: it is applicable to any flow field; it allows for the computation of the acoustics *within* complex flow regions; and, it provides a computational post-processing step for obtaining acoustic information from calculations performed using incompressible CFD codes. For this application, the input is generated by an incompressible, viscous CFD calculation, and the results are compared to results from a compressible CFD calculation. This is a joint work with Sheryl Grace.

ROGER, Michel (Ecole Centrale de Lyon, LMFA, UMR, CNRS Ecully, France)

Analytical modelling of airfoil trailing-edge and self-noise for industrial applications

The proposed paper is about analytical methods applied to airfoil self noise in two areas of interest: subsonic fans and wings with high-lift devices. The essential theoretical background is Howe's formulation of the acoustic analogy in the case of a simple or a slotted trailing edge. For a trailing edge flap, an alternative model is introduced considering the flap as a single airfoil radiating near the edge of a semi-infinite plate. The limits of the analytical approach are discussed together with the expected developments in numerical methods.

ABRAHAMS, I David (University of Manchester, UK)

Scattering by a periodic array of cracks

This talk will examine the problem of scattering of time-harmonic elastic waves by a periodic array of cracks. This is a long-standing model which has been investigated using a variety of mathematical approaches in the past. We revisit the problem and examine it by application of the Wiener-Hopf technique. In the case of out-of-plane displacements the boundary value problem is recast as a matrix Wiener-Hopf equation which, after some manipulation, is further reduced to an algebraic system of equations of easily computable form. Results will be presented for the diffracted field, and other applications of this work will be discussed.

CRASTER, Richard (Imperial College, London, UK)

Pulse scattering by subsurface cracks

Complementary techniques are used to investigate the dynamic loading of subsurface cracks in either homogeneous or inhomogeneous media; the quantities of interest such as the scattered fields and the stress intensity factors are determined. For homogeneous media these involve exact solutions utilising transform methods and the Wiener-Hopf techniques. In some cases this approach is neither feasible, due to the matrix nature of the problem, nor physically revealing, and an iterative method based on physical considerations is developed. For special loadings invariant integrals are utilised to provide non-trivial extensions of the analysis to inhomogeneous media, at least insofar as the stress intensity factors are concerned. This is joint work with D P Williams.

MOVCHAN, Alexander B (University of Liverpool, UK)

Asymptotic models of dynamic cracks propagating on an interface

We consider a 3D dynamic crack propagating along an interface in a two-phase medium. The interface surface is assumed to be flat. The reference crack occupies a half-plane, and its front propagates with a constant speed. The crack front is subject to a perturbation which depends upon both time and the space variable (along the crack front). The problem is reduced to an integral equation for the displacement jump across the interface. The asymptotic formulae for the stress-intensity factors are obtained in an integral form involving the perturbation of the crack front, applied tractions and the stress-intensity factors corresponding to the reference crack with a straight front. The asymptotic algorithm also involves the so-called weight functions representing the stress-intensity factors associated with a point load applied on the crack surface. The weight functions for a 3D dynamic crack on an interface can be obtained by solving a matrix problem of the Wiener-Hopf type.

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ORTIZ, Michael (California Institute of Technology, USA)

Application of cohesive theories to dynamic fracture and fragmentation

Advances in adaptive mesh refinement and other computational methods presently enable the simultaneous resolution of full-system fields as well as near-tip fields, with the result that the latter need not be accounted for—buried—in the fracture criterion. The explicit resolution of the near-tip fields has the far-reaching consequence that only the actual surface-separation processes need to be contemplated in the fracture criterion. In this work, those separation processes are modelled by recourse to cohesive theories of fracture and their computational embodiment, cohesive elements. As a first validation case, we have taken the dynamic drop-weight test as a convenient basis for assessing the predictive ability of cohesive models in applications involving dynamic crack growth. The numerical simulations have proven highly predictive of a number of observed features, including: the crack growth initiation time; the trajectory of the propagating crack tip; and the formation of shear lips near the lateral surfaces. The simulations therefore establish the feasibility of using cohesive models of fracture and cohesive elements to predict dynamic crack-growth initiation and propagation. A second validation case concerns the simulation of ring-expansion experiments. These experiments test the predictive ability of cohesive models in situations involving ductile dynamic fracture. Attention has been restricted to 1100-0 aluminum samples. The numerical simulations are highly predictive of a number of observed features, including: the number of dominant and arrested necks; the fragmentation patterns; the dependence of the number of fragments and the fracture strain on the expansion speed; and the distribution of fragment sizes at fixed expansion speed.

WILLIS, John R (Department of Applied Mathematics & Theoretical Physics, Cambridge University, UK)

Dynamic weight functions for a crack propagating in a viscoelastic medium

The problem is to find the stress intensity factors when a crack occupying the region $-\infty < x_1 < Vt$, $-\infty < x_2 < \infty$, $x_3 = 0$ is subjected to general dynamic loading. The medium through which the crack propagates is viscoelastic (an elastic medium being included as a special case). The intensity factors are expressed as integrals over the crack surfaces of the applied loads, multiplied by kernel functions which are called weight functions. Equations which define weight functions are set up. They yield Wiener-Hopf problems: a scalar problem for tensile loading, and a 2×2 matrix problem for shear loading. Surprisingly, both can be solved. The weight functions find use in calculating the perturbations to the stress intensity factors induced when the crack deviates slightly from being flat and straight-edged, and provide a tool for a stability analysis of the original crack, and for study of the development of "crack front disorder". This is a joint work with S Woolfries.

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CURTIS, John P (DERA, UK)

Mathematics of shaped charges

This paper presents some of the current challenges facing mathematicians at DERA in this field. It commences with a description of the process by which a shaped charge exploits the stored energy in a high explosive to form the charge liner into a hypervelocity stretching jet that can penetrate a target very deeply. The history of the shaped charge and its diverse applications are briefly reviewed. Mathematical models of the jet formation process are described. In particular the degradation mechanisms of incoherency and asymmetry are discussed. Current work on jet instability and break-up and penetration is reviewed.

DE NEUMANN, Bernard (DERA, UK)

Mathematics in Defence

This introductory talk will be concerned with stressing the importance of mathematics and mathematicians to Defence activities, both past and present, and will highlight a number of topics of current importance. The author will then go on to introduce the other speakers and their chosen topics.

FIELD, Timothy (DERA, Malvern, UK)

Twistors and electromagnetism, scattering and generation

The twistor (complex light ray) formalism for solution of the wave equation and Maxwell's equations is presented. It is demonstrated how to represent fields scattered off given charge-current distributions, and fields reflected and refracted by simple shaped bodies, in terms of associated functions defined on projective twistor space.

MCWHIRTER, John G (DERA, UK)

Blind signal separation using higher order statistics and multilinear algebra

Until recently, signal processing algorithms for the adaptive cancellation of noise from an antenna array have been based entirely on second order statistics and assumed that the spatial response of the array is known. In the last few years, techniques have been developed for blind signal separation where the array response is not known. It is assumed, instead, that the signals to be separated are statistically independent and non-Gaussian leading to the use of higher order statistics in the form of the third or fourth order cumulant tensor, for example. In this paper it will be shown how the use of multilinear algebra to handle these higher dimensional features can help to reduce the computational complexity.

BRAACK, Malte (INRIA, France)

Application of weighted residual error estimates to adaptive mesh refinement

We apply weighted a posteriori error estimation to the finite element discretization of the incompressible Navier-Stokes equations and the low-Mach-number approximation for reactive compressible flow. Using information from a appropriate discrete dual problem we control the discretization error of a functional of the solution. For the non reactive case, typical functionals are drag and lift coefficients. For the simulation of combustion processes, we control, e.g., particular species mass fractions.

GILES, Michael B (Oxford University, UK)

Improved lift and drag estimates using adjoint Euler equations

We show that error analysis using the numerical solution of an appropriate adjoint PDE can be used to improve the order of accuracy of integral functionals obtained from CFD calculations. Numerical results obtained using a standard second order accurate approximation of the quasi-1D Euler equations demonstrate that one can achieve fourth order accuracy for the integrated pressure. Similar improvements are also obtained for 2D applications.

MACHIELS, Luc (MIT, USA)

A posteriori finite element bounds for output functionals of the incompressible Navier-Stokes equations

We propose a new finite element *a posteriori* error control strategy for the incompressible Navier-Stokes equations. The technique provides lower and upper bounds for the output of interest that are inexpensive to compute, rigorous, quantitative, and sharp; furthermore, the bound gap permits a local (elemental) decomposition suitable for adaptive subsequent refinements. The method considerably generalizes earlier techniques in that we obtain quantitative constant-free bounds - contrary to earlier explicit techniques - for the output of interest - contrary to earlier implicit techniques.

SÜLI, Endre (Oxford University, UK)

A posteriori error estimation for stabilised finite element approximations of hyperbolic problems

We develop the *a posteriori* error analysis of stabilised finite element approximations of scalar hyperbolic equations, including the streamline diffusion method and the least-squares stabilised finite element method. In particular, we discuss the question of error estimation for linear functionals, such as the outflow flux and the local average of the solution. The theoretical results are illustrated by numerical experiments. This is a joint work with Rolf Rannacher, University of Heidelberg and Paul Houston, University of Oxford.

BÜRGER, Raimund (University of Stuttgart, Germany)

Model equations for sedimentation-consolidation processes

We develop a general phenomenological theory of sedimentation-consolidation processes of flocculated suspensions, which are considered as mixtures of two superimposed continuous media. Following the standard approach of continuum mechanics, we derive a mathematical model for these processes by applying constitutive assumptions and a subsequent dimensional analysis to the mass and linear momentum balance equations of the solid and liquid component. In two or three space dimensions, solvability of the resulting equations depends on the choice of phase and mixture viscosities.

In one space dimension, however, this model reduces to a quasilinear strongly degenerate parabolic equation, for which analytical and numerical results are available. The application of this theory to batch and continuous sedimentation-consolidation processes is illustrated.

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DIEHL, Stefan (Centre for Mathematical Sciences, Lund University, Sweden)

Uniqueness problems in the one-dimensional modelling of continuous sedimentation

The industrial process of continuous sedimentation of solid particles in a liquid takes place in a clarifier-thickener unit (large tank), which has one feed inlet (middle of tank) and two outlets (top and bottom). It can be modelled in one dimension (depth of tank) by a non-linear conservation law with a point source and discontinuous flux function. The problems of non-uniqueness of solutions at the source (inlet) and the boundaries (outlets) are resolved by a generalized entropy condition, which is illustrated and motivated by examples with varying cross-sectional area.

EVJE, Steinar (University of Bergen, Norway)

Finite difference schemes for degenerate convection-diffusion equations with applications in simulation of sedimentation processes

We establish convergence of finite difference schemes for nonlinear possibly strongly degenerate convection-diffusion equations of the form $\partial_t u + \partial_x f(u) = \partial_x^2 K(u) + q(u)$, $K' \geq 0$, $q' \leq 0$, $u(x, 0) = u_0(x)$. Such models have been used in the study of certain sedimentation processes. We refer to the system above as strongly degenerate since $K(u)$ is only required to be nondecreasing. Consequently solutions can be discontinuous and are in general not uniquely determined by their data. In particular, we want to construct first and second order accurate schemes whose properties are consistent with the properties of the true solutions. For this purpose, it is useful to work with the (narrow) class of so-called *BV entropy weak solutions*. A recent result of Wu and Yin states that for this class of solutions, the problem above is well-posed. Compared with the convergence analysis well known from the conservation law theory, the new aspect which must be taken into account here, is to verify that the discrete diffusion term possesses the regularity known to hold for *BV entropy weak solutions*.

EWING, Richard E (Institute for Scientific Computation, Texas A&M University, USA)

Simulation of contaminant transport involving two-phase flows

Three basic problem areas have dominated much of the recent research in reservoir simulation. First, one must obtain an effective model to describe the complex fluid/fluid and fluid/rock interactions that control recovery processes. This includes the problem of obtaining accurate reservoir descriptions at various length scales and including the effects of this heterogeneity in the reservoir simulators. Next, one must develop accurate discretization techniques that retain the important physical properties of the continuous models. Finally, one should develop efficient numerical solution algorithms that utilize the potential of the emerging computing architectures. We will discuss recent advances in each of these three areas.

HESSE, Christian (Mathematics Institute A, University of Stuttgart, Germany)

A new methodology for modeling particle sedimentation in fluids

In this talk we discuss the usefulness of a model based on non-linear Langevin-type equations with configuration-dependent parametrization for the study of particle sedimentation in viscous fluids. By a method that utilizes measure-valued stochastic processes, we study system dynamics and address issues such as parameter estimation and model-fitting. We also compare our results to previous modelling efforts, such as Kynch theory and its extensions.

KARLSEN, Kenneth H (Department of Mathematics, University of Bergen, Norway)

Numerical methods for the simulation of the settling of flocculated suspensions

For one space dimension, the phenomenological theory of sedimentation of flocculated suspensions yields a model that consists of an initial-boundary value problem for a second order partial differential equation of mixed hyperbolic-parabolic type which may possess discontinuous solutions. Due to the mixed hyperbolic-parabolic nature of this model, difficulties arise if one tries to solve this model numerically by classical methods for parabolic partial differential equations. Numerical methods based on naive finite difference approximations may work well for smooth solutions but can give wrong results when discontinuities are present. In this paper we present and elaborate on numerical methods which *can* be used to correctly simulate this model. Included in our discussion are finite difference methods and methods based on operator splitting. In particular, the operator splitting methods are used to simulate the settling of flocculated suspensions.

SCHAFLINGER, Uwe H (University of Technology, Graz, Austria)

Resuspension phenomena in laminar flows

Resuspension is a process by which an initially settled layer of heavy, non-Brownian particles in contact with a clear fluid above is set into motion by a laminar shear flow. It has been observed that even at low Reynolds numbers at least part of the sediment layer will resuspend. Based on a theoretical model several uni-directional flows, e.g., a plane Couette flow, a plane film flow, a 2D Hagen-Poiseuille channel flow, and a laminar pipe flow were investigated successfully. Measurements of the resuspension height in a 2D Hagen-Poiseuille channel flow are in overall agreement with the theoretical predictions. The data show, however, considerable scatter that was attributed to the difficulties in performing the measurements and to the presence of interfacial waves. Also, if the flow rate was small, the observed pressure drop was slightly larger than predicted. In the case of relatively large flow rates the measured pressure drop was surprisingly much smaller than predicted by theory. A linear stability analysis shows that a 2D Hagen-Poiseuille channel flow is always unstable to interfacial waves and that two different convective instabilities can coexist within a certain range of parameters. A sub-sequent nonlinear study of the interfacial instabilities reveals that the waves indeed influence the pressure drop as observed experimentally.

TORY, Elmer M (Mount Allison University, Canada)

Stochastic simulation of sedimentation

The three-parameter Markov model for sedimentation uses the mean, variance, and autocorrelation of particle velocities. These three parameters are assumed to be functions of a concentration parameter that is a convolution of local concentrations with a Gaussian kernel. Using this model, we simulate the settling behaviour of a very dilute dispersion. The simulation follows the general scheme of Hesse and Ramos, but uses a stochastic Runge-Kutta method developed by Honeycutt and adapted for sedimentation by Tory et al. The simulated results capture features of settling tests that are not predicted by Kynch's theory. This is a joint work with Robert A. Ford.

BETTESS, Peter (School of Engineering, Durham University, UK)

Solving short wave problems using special finite elements

The solutions to the Helmholtz equation in the plane are approximated by systems of plane waves propagating in all possible directions. The aim is to develop finite elements capable of containing many wavelengths and therefore simulating problems with large wave numbers without refining the mesh to satisfy the traditional requirement of 10 nodal points per wavelength.

DARVE, Eric (Universite Pierre et Marie Curie, Paris, France)

Fast multipole method: Application to the Maxwell equations

The application of a dense ($N \times N$) matrix to an arbitrary vector can be done with $O(N^2)$ operations. Codes based on an integral formulation lead to such matrices and this $O(N^2)$ complexity is one of the difficulties encountered in large-scale computations. This is why integral equations have had a limited use so far and are often avoided whenever possible. For example, finite element and finite difference methods can be viewed as a way of sparsifying the matrix. Most iterative techniques used to solve linear systems involve the computation of matrix vector products and the construction of a recursive set of vectors. Compared to a direct solver in which the inverse of the matrix is computed ($O(N^3)$ operations) this means a significant reduction in the complexity ($O(N_{iter}N^2)$ operations). For the Helmholtz/Maxwell equations, the special nature of the integral operator, its oscillatory nature for example, makes it necessary to derive a specific scheme that uses its particular analytical structure. It requires a fairly subtle mathematical apparatus but once constructed this algorithm proves to be extremely efficient. Complexity of $O(N_{iter}N \log N)$ or $O(N_{iter}N \log^2 N)$, depending on the particular implementation of the Fast Multipole Method (FMM), is achieved. In this talk we will give a general overview of multipole methods and the specific derivation of the FMM for the Maxwell case. We will state an error estimate which is a refinement of results obtained previously. We will focus the talk on the numerical results obtained with an integral code which uses a Combined Field Integral Formulation, a SPAI preconditioner and the FMM. Those numerical results demonstrate the usefulness of this method.

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LEVY, Mireille F (CLRC Rutherford Appleton Laboratory, UK)

Marching methods for electromagnetic scattering computations

We present two marching methods which make it possible to solve scattering problems for large objects on desktop computers. The vector parabolic equation is a paraxial version of Maxwell's equations which solves for the fields by marching them along a preferred direction. The full bistatic scattering is obtained by rotating the paraxial direction. The current marching technique is an iterative solver for the integral equation giving the electric current, with remarkably good convergence properties. A dual-surface integral equation is used to eliminate resonance problems. Both methods are applied to RCS calculations at microwave frequencies. This is joint work with A.A. Zaporozhets.

MURPHY, John A (British Aerospace, Sowerby Research Centre, UK)

A review of computational electromagnetics in the aerospace sector

To address requirements such as radar scattering, electromagnetic hazards and lightning strike, Computational Electromagnetics (CEM) has experienced significant growth. Despite this, CEM is still a relatively immature discipline and problems often need to reflect geometric detail, varying geometrical scales, and are computer-intensive. The development areas span electromagnetically larger problems, improved representation of the engineering problem and efficient pre and post-processing. Research efforts need to be balanced between improving the electromagnetic models, particularly for accurate predictions at high frequencies, and enabling the end-user engineer to handle the simulation complexity, which spans developments in many pre and post-processing tools.

PARROTT, Kevin (University of Greenwich, UK)

Applications of the adjoint method to high frequency electromagnetic computations

Quantities related to a (weighted) energy flux through a surface in space occur in the determination of the input-output characteristics of a microwave wave-guide, and the scattering properties (RCS) of an object. When edge finite elements are used to discretize the electro-magnetic field calculation the appropriate surface values of the fields are not available. Some form of interpolation scheme has to be used to obtain the desired quantity but this is difficult to analyze. The adjoint method of Wheeler (later analyzed by Babuska et al) avoids these difficulties and can improve accuracy. Its application is described for these calculations, with results for 3-D model problems. This is joint work with Peter Monk, University of Delaware.

WALKER, Simon P (Imperial College, London, UK)

Time domain integral equations for high frequency computational electromagnetics: Computational issues, costs and performance

In this paper we review briefly the main issues which give rise to the fearsome computational costs, and the cost scalings with frequency, of high frequency electromagnetic scattering computations. The origins of the cost scaling of the main alternative approaches are considered, with particular emphasis on the integral equation time domain (IETD) approach. Recently developed methods to reduce these are then described, and results are presented which show that significantly reduced cost scalings in the IETD approach can be achieved, and accurate full-field solutions obtained on multi-wavelength bodies. This is joint work with M J Bluck, Imperial College.

SVANSTEDT, Nils (Chalmers University, Sweden)

Two-scale limits and mean fields for flows

We consider the Navier-Stokes system with small viscosity. For highly oscillatory fluids we prove the existence of a two pressure limit. As a benefit the analysis shows that length, time, velocity and viscosity scale as predicted by Kolmogorov. In systems where the periodicity is relaxed a straightforward averaging over the local spatial scale yields the mean field which turns out to satisfy the Euler equation. A typical situation is classical Rayleigh-Bernard convection where experiments have shown that highly irregular behaviour presumably is caused by the underlying the mean field.

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ZULKIFLE, A K (University of Strathclyde, Glasgow, UK)

Curing Simulation by Autoclave Resin Infusion

This talk deals with the modelling and simulation of resin flow, heat transfer and the curing of a multilayer thermoset composite by the resin film infusion process. For approximately isothermal flows, the model is based on Darcy's law and Stoke's equations where a similarity solution is obtained and subsequently used in a two-dimensional convection-diffusion heat equation coupled with a rate of cure equation. A finite difference scheme is applied to the energy equation on a moving grid and simulations for varying thicknesses and number of plies are performed.

LACEY, Andrew A (Heriot-Watt University, Edinburgh, UK)

Modelling moisture and temperature variation in sugar silos

The distribution of heat and moisture in sugar stored in large silos affect the quality and consistency of the sugar and the risk of dust explosions: too much moisture causes the quality to deteriorate and produces caking but too little greatens the chance of an explosion. A simple mathematical model for both temperature and water content, valid over a timescale of a few months, is derived, assuming forced convection through the silo. This problem was tackled during the 32nd European Study Group with Industry (Lyngby, 1998).

PARKER, David F (University of Edinburgh, UK)

Surface layers in electrochemical machining problems

Electrochemical machining (ECM) is usually modelled as a moving boundary problem for Laplace's equation with the erosion rate of the anode surface governed by local current density. This model assumes charge neutrality within the fluid electrolyte. While this is appropriate away from surfaces, nonequilibrium layers occur nearby, in which species diffusion is important. The associated potential drop, known as 'overpotential', significantly affects the moving boundary problem. Appropriate scaling and matching of asymptotic expansions determines this overpotential, including surface-curvature effects. Combined with a boundary integral implementation for Laplace's equation, predictions for a number of surface shaping and smoothing problems are computed. This is joint work with G J Darling, Edinburgh Parallel Computing Centre.

ROBBINS, Chris (University of Strathclyde, UK)

Discrete element simulation and its application to fire safety and evacuation

The discrete element method is a gridless approach to simulating the motion of granular materials. Traditional applications have considered inert materials: wheat-grain, rocks, etc., however, the method can be extended to "intelligent" grains that respond to a motive force other than gravity and display purpose. Adding these characteristics allows a granular simulation of a crowd people to be performed where the motive forces are due to individual desires such as the wish to move to a particular location. Interaction causes a slowing down of motion in areas where crowd densities are high, simulating the effects seen in real crowds. As a demonstrative example, an evacuation of a Boeing 737 during a fire is simulated. This includes approximate environmental feedback from the smoke and predictions of the number of passengers incapacitated are made.

WILSON, Stephen K (University of Strathclyde, Glasgow, UK)

Some industrially-motivated problems involving thin fluid films

Many industrial situations involve thin fluid films. In this talk we shall describe mathematical models for several such situations and the novel features they reveal. In particular, we shall consider drying paint layers, coating flows over rotating substrates and the expansion and contraction of a vapour bubble in nucleate boiling.

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AUSTIN, Daren (Oxford University, UK)

Mathematical models of infectious disease: From populations to individuals

The burden of infectious disease continues to present a major challenge to human and animal health. The use of mathematical models to further the understanding of the persistence and control of infections presents many challenges on all scales from populations to the individual. In this talk I will discuss how the contributions made by the field of mathematical biology contribute to our current understanding. On the largest scale, the dynamics of childhood infections and the potential impact of vaccination show considerable complexity which only now is beginning to be unravelled. At smaller hospital scales, models of infection in small populations present new challenges requiring both stochastic and deterministic techniques. Finally we will consider the advances made in our understanding of within-host infections such as HIV, and their effective management using anti-retroviral therapy.

COVENEY, Peter V (Centre for Computational Science, Queen Mary and Westfield College, University of London, UK)

Renormalisation group theory and multiscale modelling problems

So-called mesoscale modelling and simulation methods have attracted much interest recently. These approaches aim at providing a description of the behaviour of generally complex systems on length and time scales which are intermediate between the microscopic (atomic/molecular) and macroscopic (continuum) levels. Many complex physical phenomena are controlled by processes occurring on this mesoscale. We discuss the application of renormalisation group ideas to models of cluster formation in nucleation and growth processes, and to the derivation from molecular dynamics of multiscale techniques for the description of complex fluid hydrodynamics.

COWAN, Jack D (Mathematics Department, University of Chicago, USA)

Neural networks

A short account will be given of mathematical aspects of the modelling of nerve cells or neurons, and neural networks. Two differing applications will be described, the first devoted to brain modelling, the second to artificial intelligence. We will introduce the mathematical description of neurons as devices that emit current pulses in response to incoming signals and describe the various mathematical approaches which are used to represent and analyze their properties. We will then look at networks of such devices and describe various methods for analyzing the new phenomena which emerge when large numbers of these devices are coupled together into re-entrant circuits or networks. In so doing we will touch on various mathematical topics such as analyzing nonlinear differential equations via singular perturbation, solving the cable equation on branched tree-like structures, and bifurcation theory in the presence of symmetry groups. We will then introduce the study of neural networks for artificial intelligence and give an account of how such networks are used in such areas as machine learning, image processing, and statistical explorations of data bases.

HODGES, Stewart (Warwick Business School, University of Warwick, UK)

What's going on in financial derivatives?

Financial derivatives (futures, options and other even more exotic kinds of contracts) are seldom out of the news for long, and often appear to be synonymous with financial disaster. This talk will review in general terms, the nature of the methods used to value these instruments and to control their risks. It will discuss the weaknesses of these techniques and describe the kinds of research currently going on to develop risk measures which are more accurate, and hedges which are more robust.

SINAI, Yakov G (Princeton University, USA)

Recent progress in theoretical and statistical hydrodynamics

Mathematical hydrodynamics studies mostly properties of solutions of Navier-Stokes and Euler equations. Since the problems are fundamental solutions should be enough simple to be of general importance and should combine mathematical rigor with physical intuition. Recently some progress was achieved in the existence and uniqueness problems for Navier-Stokes system with periodic boundary conditions. Another set of problems where there was some success recently concerns Burgers equation equation with random forcing. All these topics will be discussed during the talk.

YOUNG, Lai-Sang (University of California, Los Angeles, USA)

Mathematical theory of chaos

Lyapunov exponents and entropy are two different ways of measuring chaos in finite dimensional dynamical systems. Comparing them leads to an understanding of the fractal dimension of sets, of strange attractors and of the rate of escape from transient chaos. These rates are related to the speed of mixing and other statistical properties of dynamical systems. This talk is a survey of known results including very recent work.

FIORENTINO, Giuseppe (Dipartimento di Matematica - Università di Pisa - Italy)

Numerical solving of polynomial systems

We introduce a package for reliable polynomial computations that can isolate, approximate up to any number of digits or count all the roots of a univariate polynomial in a given subset of the complex plane. The package has been designed with efficiency and accuracy as main goals and is tailored to face the extreme numerical difficulties arising from the symbolic preprocessing of real life problems.

Numerical experiments show that the method provides a reliable and fast tool for solving univariate polynomial equations and polynomial systems. The speed up factors, with respect to current available software, arrives up to several thousands. This is joint work with Dario Andrea Bini.

GONZALEZ-VEGA, Laureano (Universidad de Cantabria, Spain)

Integrating symbolic and numeric computations in CAGD

One of the main problems arising in the manipulation of parametric surfaces in computer aided geometric design is the finding of efficient algorithms for computing the implicit equation of surfaces parametrized by rational functions. This is due, for example, to the fact that, if for tracing the considered surface the parametric representation is the most convenient, to decide in an efficient way the position of a point with respect to the surface considered, the implicit equation is desired. Two main difficulties are encountered when trying to use the usual elimination techniques offered by Computer Algebra to deal with the variable elimination problems mentioned before. For example the implicitation of a rational surface defined by $x = \frac{X(s,t)}{W(s,t)}$, $y = \frac{Y(s,t)}{W(s,t)}$, $z = \frac{Z(s,t)}{W(s,t)}$ appearing in a real-world problem is difficult to achieve by applying directly resultants or Grobner Bases because, first, it is usually a very costly algebraic operation and, second, the coefficients of the polynomials involved into the parametrization are usually floating-point real numbers. It will be shown how these difficulties are currently overcome by taking into account that, in general, a concrete object to model is made by several hundreds (or thousands) of small patches, all of them sharing the same algebraic structure: for such an object a database is constructed containing the implicit equation of every class of patch appearing in its definition. This database must also contain the inversion formulae (giving the parameters in terms of the cartesian coordinates) and must be pruned to avoid specialization problems. Moreover the database for a specific object is kept into a bigger and general database for a further use.

MOURRAIN, Bernard (INRIA, SAGA, FRANCE)

Integrating symbolic and numeric Computations. Applications to robotics and computational biology

In this presentation, we will focus on methods using linear algebra tools for solving polynomial equations. The first step consists in reducing the root-finding problem to eigenproblems, by exploiting the properties of the operators of multiplication in the quotient algebra. The second step consists in constructing these multiplication matrices from resultant matrices. The next step consists in exploiting the structure of these matrices, in order to devise efficient algorithms. We will show the applicability of this approach to problems involving polynomial equations with approximate coefficients. We will also illustrate these tools by explicit experimentations, with the library ALP devoted to symbolic and numeric algebra for polynomials. Finally we will end with some applications to robotics problems, to calibration problems in computer vision, to molecular biology problems or to signal processing.



TRAVERSO, Carlo (Department of Mathematics, Pisa, ITALY)

Integrating symbolic and numeric computations with the PoSSo library

We describe the features of the FRISCO C++ library that allow efficient and safe computation of Groebner bases using floating coefficients, and the tools that allow the study of the intrinsic conditioning of the Groebner basis derived from the input data. The tools include different floating types (hybrid modular+floats, double bigfloats) and infinitesimals. Some preliminary experimental findings are discussed; especially significant is the apparent superiority of algorithms based on linear algebra techniques with respect to Buchberger-like algorithms as far as numerical stability is concerned.

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KIDA, S (National Institute for Fusion Science, Nagoya, Japan)

DIA theory: Principle and applications

Although individual instantaneous flow fields of turbulence vary chaotically, the ensemble or temporal average of them exhibits rather robust and universal structures such as the Kolmogorov energy spectrum at small scales and the logarithmic velocity profile in wall turbulence. It is tempting then to try deriving such universal properties from the Navier-Stokes equation which is believed to describe turbulence properly. As one of the most promising approximation theories, we discuss here the direct interaction approximation (DIA), the idea of which dates back to Kraichnan (1959). A special attention is paid to the basis of DIA which has often been confused even among experts.

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CLEARY, Paul W (CSIRO Mathematical and Information Sciences, Australia)

Deterministic and statistical models for industrial granular flows

In principle, industrial granular flows (e.g. flow of rocks in a mill, filling of an excavator bucket, discharge of a silo), can be predicted by deterministic methods. Each particle obeys Newton's laws and undergoes collisions which can be modelled. Completely deterministic solutions would require perfect knowledge of the particle shapes, material properties and the initial configuration (positions, velocities and spins). Statistical methods allow us to characterise distributions of these properties and provide ensemble averages of predicted quantities over these distributions. They also play a vital role in extracting useful information from the vast body of data produced by deterministic methods.

GLASBEY, Chris A (Biomathematics and Statistics Scotland, UK)

Deterministic and statistical approaches to image analysis

Three aspects of image analysis will be considered where both deterministic and statistical methods have been applied: tomographic reconstruction from projections, template matching, and model fitting by function minimisation. In tomography, with PET and SPECT data, deterministic and statistical image reconstruction algorithms will be compared. Then, the application of deterministic and stochastic templates to images of man-made and natural objects will be contrasted. Finally, as image analysis often leads to hard optimisation problems, the uses of simulated annealing and variational methods will be discussed.

JOLIFFE, Ian T (University of Aberdeen, UK)

Statistical modelling in atmospheric and other environmental sciences

Since all models are wrong the scientist cannot obtain a "correct" one by excessive elaboration' - Box (1976). For some complex systems, however, such as the atmosphere, elaborate models are necessary. Deterministic models, though wrong, can provide excellent explanations and predictions at some spatial and temporal scales. At other scales the introduction and modelling of stochastic variability can bring advantages. A number of ways in which statistics can help in analysing complex physical systems including, but not restricted to, the atmosphere will be outlined. The emphasis will be on potential applications of recent statistical developments.

SANDLAND, Ron (Chief, CSIRO Mathematical and Information Sciences)

Deterministic or stochastic? Choosing a modelling approach that works

Modelling of processes in industries such as Manufacturing can greatly improve understanding of operational characteristics and hence result in gains in quality and productivity. But how do we model such processes appropriately?

Deterministic modelling requires a sound understanding of the physical, chemical, biological processes that constitute the systems being modelled. A statistical approach may be appropriate when the underlying processes are too complex to model explicitly, or when the system includes inherently stochastic components (eg sampling variation).

I shall approach this interface from the statistical side using examples to illustrate general principles for choosing the modelling approach.

APOSTOLICO, Alberto (Purdue University, USA and University of Padova, Italy)

Algorithms for detecting unusual words

The problem of characterizing and detecting unusual events such as recurrent subsequences and other streams or over/under-represented words in sequences arises ubiquitously in diverse applications and is the subject of much study and interest in Computational Molecular Biology. There, words that are, by some measure, typical or anomalous in the context of larger sequences have been implicated in various facets of biological function and structure. The detection of unusual words on a massive scale poses interesting methodological and algorithmic problems, some of which are reviewed in this talk, together with related implementations and empirical results.

GIANCARLO, Raffaele (University of Palermo, Italy)

Hidden Markov models in molecular biology

Hidden Markov Models (HMM's for short) are a very powerful tool to (a) characterize common patterns and features in a family of strings and (b) measure how well a new string fits those patterns and features. This is very well illustrated by the use of HMMs in Automatic Speech Recognition. Indeed, most large dictionary speech recognition systems use HMMs at the most basic stages of acoustic recognition. In the past few years, HMMs have found also use in computational problems in Molecular Biology, mostly for Protein Sequence Analysis. In this talk we will briefly introduce HMMs and discuss some of the algorithmic problems related to them. Then, we will show how they are applied to Profile Alignment problems in Computational Biology.

RAVI, R (Carnegie Mellon University, USA)

A set covering formulation of the epitope selection problem

Selecting a small number of epitopes (sequence-specific binders) that can distinguish among a given catalog of protein sequences is an interesting computational problem that precedes the design of a chip that can be manufactured for this purpose. We show how to formulate this as a set covering problem and describe some preliminary results of our approaches to solve an instance.

ARCHIBALD, Tom (Business Studies, The University of Edinburgh, UK)

Comparison of linear programming and dynamic programming on large scale reservoir optimization problems

Reservoir control has been a classic problem in Operations Research since Masse first modeled it in 1946. However problems involving realistic systems with many reservoirs connected together have proved difficult to solve due to the computational requirements. The advent of parallel computers and the success of decomposition methods have led to more work on this problem recently. This talk looks at four different approaches to solving the reservoir control problem. Two involve linear programming and two involve dynamic programming. The paper compares computational and other characteristics of the approaches. This is a joint work with Ken McKinnon and Lyn Thomas.

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BAXTER, Rob M (EPCC, The University of Edinburgh, UK)

Well, what can you deliver?

Contract manufacturing is a tough business. Margins are low, pressure is high and flexibility is essential. If a customer phones up and says "I want to change next week's order from 10,000 Widget Assemblies to 20,000. Can you deliver?", you need to know the answer. If you don't know, or guess wrong, your customer will go elsewhere. Working with three end-users from Scottish manufacturing, EPCC's recently completed Industrial Process Optimisation (IPO) project set out to provide production planners with a tool to answer questions like this quickly and optimally. A key aim was to develop a tool which would tell the planner the "best" set of units to build with the available stock — "I know I don't have the materials to meet these orders exactly, but what can I deliver?" This talk gives an overview of the completed IPO optimising materials planning system.

KALLIO, Markku (Helsinki School of Economics, Finland)

Parallel computing for large-scale convex optimization

We discuss a recent solution technique for large convex optimization models with differentiable objective and constraint functions. The method is based on saddle point computation of the standard Lagrangian. In each iteration the update directions for primal and dual variables are determined by gradients of the Lagrangian. These gradients are evaluated at perturbed points which are generated from current points via auxiliary mappings. The resulting algorithm suits massively parallel computing. Using Cray T3E parallel computer, we demonstrate the approach using a multi-stage stochastic LP for forestry planning as well as several versions of a nonlinear model for asset-liability management in a pension insurance company.

SLOAN, Terry M (EPCC, The University of Edinburgh, UK)

Experiences in extracting useful information from data

It is widely accepted that increasing numbers of organisations wish to make more use of their operational data. Across the spectrum from financial enterprises to academic research institutions there is a wealth of such data and the desire to gain extra benefit from it. However for many the question remains how exactly to do this. In recent times, data mining in its various guises has gained much credibility as a possible mechanism for doing this. There have been successes but the techniques are not always applicable. Issues such as incomplete data, insufficient data volumes and unclean data have all contributed to occasions when knowledge discovery methods cannot be applied easily or efficiently. EPCC has helped a number of clients extract extra benefit from their operational data. The methods utilised have not always been data mining based nor "rocket science" but they have been appropriate to the task at hand and within the means of the clients. As such they have helped the client get that extra information they wanted from their data even when their data was incomplete or not easily suited to data mining. In this talk I will outline some of our experiences on such projects. These projects used a range of techniques, from typical data mining methods such as decision trees to statistical modelling and knowledge based systems - in effect using the methods which were able to get information out given the constraints of the data and application. In this way I hope to show that as with all tasks, you get the most benefit when you use an appropriate tool.

BOOTH, Stephen P (EPCC, The University of Edinburgh, UK)

Zero to infinity

Parallel computers are used extensively to simulate systems from many branches of physics at many different length scales. This talk examines two different simulations from opposite physical extremes. Lattice gauge simulations (UKQCD consortium) simulating the smallest of sub-atomic particles. Galaxy formation (VIRGO consortium) simulating the large scale structure of the universe. Both of these are "grand challenge" problems that require powerful supercomputers and both consume large amounts of computer time on the T3E system at EPCC. The different nature of these two problems and the particular difficulties associated with the parallel implementation of each one are discussed in detail.

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LAVANTE, Ernst von (University of Essen, Germany)

Numerical simulations of vortical flows using parallel computers

In many realistic applications of computational fluid dynamics (CFD), the flows under consideration display significant, or even locally dominant, vortical structures. They are mostly geometrically and physically complex, making their phenomenological description difficult and their numerical simulation demanding. These types of flows could be compressible or incompressible, but they are almost always to be considered as three-dimensional, viscous and unsteady, with possibly some additional physical features, such as, for example, non-equilibrium chemistry. The relatively large vortices make the application of large eddy simulation methods (LES) a promising alternative to the more common turbulence models. However, in this case, the larger scale eddies in the boundary layer have to be captured by the scheme, increasing the requirements for spatial and time-wise resolution even further. The computational grids used in these cases consist of several million nodes or cells that have to be advanced in time by many hundred thousand iterations. Clearly, only the most capable computer systems available today, such as the massively parallel computers, will be able to carry out these computations in reasonable time. In the present work, numerical simulations of flows of the above type are discussed. These include several typical industrial configurations, such as flow meters or critical flow metering nozzles, as well as a model of a supersonic combustion chamber. The task of predicting these flows is parallelized using the so called domain decomposition technique. The present code is implemented on several parallel computer systems including a cluster of workstations, smaller scale parallel computers (Parsytec, NEC Cenju) and massively parallel systems (Cray T3D, T3E and IBM SP2). The problems of efficient parallelization and code optimization will be discussed in detail. Special emphasis will be put on the treatment of numerical issues. The results of the present simulations will be validated and verified using corresponding experimental data or results of other investigators. The unsteady character of the resulting flow simulations will be demonstrated by showing their video records.

OPENSHAW, Stan (University of Leeds, UK)

Developing and applying smart geographical data mining tools to GIS databases

Current data mining software seems almost totally helpless at handling complex geographically referenced databases where location is an important attribute. It is noted that GIS data contains three types of information: map location, time location, and various multivariate attributes. Patterns and relationship can involve any or all of these data types and they can interact. The talk outlines the development of computationally intensive geographical data mining methods and illustrates their application with the analysis of health and crime data. Here the role of HPC is essentially to power the data mining activities thereby also establishing benchmarks that are subsequently presented as targets for smarter methods to try and beat. The results are presented via animation of the search processes as a means of aiding end-user understanding. This is a joint work with Ian Turton and James Macgill.

WESTHEAD, Martin (EPCC, The University of Edinburgh, UK)

Intersim: Large scale simulation of internet traffic

The growing scale and complexity of the Internet is leading to increasing problems in the design and modification of its protocols, algorithms, and hardware and software configurations. Current design practices are critically inadequate and new techniques and tools must be brought to bear. Current protocol design methodology makes extensive use of simulation in order to verify the correctness, and assess the performance of prototype designs. However these simulators are often small parts of design projects and as such are typically limited to modelling small systems with only the protocol itself under consideration. The existence of so many non-standard simulators means that comparison between alternative solutions to a problem becomes very difficult. Frequently, the first real test of the performance and scalability of an Internet protocol or algorithm has been when it has been deployed on an operational network. This has led to a situation in which networks are fragile, unpredictable, and hard to maintain. The Intersim project aims solve these problems by providing a standard modular simulator which will use HPC techniques to dramatically increase the scope and scale of network models that can be simulated. This paper will present preliminary result from this work.

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CATLOW, Richard (The Royal Institution of Great Britain, UK)

UK scientific computing in the Petaflop Era

The UK scientific community has an excellent track record in the successful exploitation of High Performance Computing, as shown by the successful exploitation over the last five years of the MPP T3D/E resources at EPCC. The talk will summarise recent scientific developments and trends in the use of HPC by UK scientific users, and will highlight notable recent achievements in fundamental and applied science. We will then consider the scientific opportunities that will be opened up by petaflop computing and the ways in which these might be exploited by the UK community. We will consider the nature of the scientific infrastructure needed to support effective use of petaflops computing.

HEGGIE, Douglas (Mathematics, The University of Edinburgh, UK)

Status of the GRAPE (GRAvity PipELine) project

The GRAPE (GRAvity PipELine) project has run at the University of Tokyo since 1989. It has resulted in the construction of a series of special-purpose hardware devices for summing inverse-square forces, and similar tasks. For certain problems in astrophysics GRAPE is now essential for competitive research. This talk gives a user's view of the existing hardware, and prospects for the next generation: a 200 Teraflop version by 2001.

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HAINES, Keith (Meteorology, The University of Edinburgh, UK)

Global ocean circulation modelling using satellite data

Weather forecasting models regularly require large amounts of observational data to provide initial conditions from which to launch forecasts, typically up to 10 days ahead. Boundary conditions such as ocean temperatures are normally kept fixed during these forecasts. However if it were possible to forecast sea surface temperatures (SST) for many months ahead (eg. for El Nino years) these SST may be used in predicting those aspects of the weather which are sensitive to them. Ocean models also require large amounts of ocean data if they are to be used for such prediction. Since 1991 satellite altimeters have been flying which give an accurate measure of sea level globally every 10 days. These sea level maps can be used to infer currents and to initialise ocean circulation models for prediction. We report forecast experiments using the OCCAM global ocean model run on the T3D at Edinburgh, assimilating satellite altimeter data from 1993-1995. These results contribute to international programs such as GOOS (Global Ocean Observing System) and GODAE (Global Ocean Data Assimilation Experiment).

PALMER, Tim (European Centre for Medium-Range Weather Forecasts (ECMWF), UK)

Predicting uncertainty in weather and climate forecasts

The formal solution to the problem of predicting uncertainty in weather and climate prediction can be posed in terms of the Liouville equation for deterministic systems, or the Fokker-Planck equation, taking uncertainties in model formulation into account. In practice the problem is approached using ensembles of integrations of the deterministic weather and climate prediction models, perturbing both initial conditions and model formulation. The ensemble prediction system of the European Centre for Medium Range Weather Forecasts is described, and examples of the resulting probabilistic forecast products are shown, both on daily and seasonal timescales. Methods to evaluate these probabilistic forecasts are discussed. By feeding output from probability forecasts to user-specific decision models, it is shown that that probability forecasts of weather and climate have greater economic value than corresponding deterministic forecasts.

SMITH, Douglas A (EPCC, The University of Edinburgh, UK)

Increasing the efficiency of the UK Meteorological Office unified model

The United Kingdom Meteorological Office has its own forecasting code known as the Unified Model. It is used to predict both the coming week's weather and the climate in hundreds of years time. Obviously predicting yesterday's weather today is a waste of time and for this reason UKMO uses one of the most powerful supercomputers in the world. Over the past year EPCC has been working with UKMO on parts of their weather prediction codes. I discuss single processor optimisation of the code modelling the effect of solar radiation on the weather and the parallel load balancing of the code modelling the advection of tracers through the atmosphere.

BULL, Mark (EPCC, The University of Edinburgh, UK)

HPC programming models and languages

Just as important as hardware are the programming models and languages used to implement HPC applications. This area is showing signs of reaching a stage of maturity, with standardisation efforts coming to fruition in recent years. This talk will outline the basic programming models used in HPC, and describe how these are implemented in current language and library standards. Again, future trends in this field will be discussed.

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HENTY, David S (EPCC, The University of Edinburgh, UK)

Case studies in HPC

In this final session, we will look at particular applications areas including global ocean circulation modelling and astrophysical simulations of the evolution of the entire universe. We examine how HPC is used in these areas and the impact that it has had.

MINTY, Elspeth (EPCC, The University of Edinburgh, UK)

Introduction to High Performance Computing

High Performance Computing (HPC) is an increasingly important tool in a wide range of scientific and other disciplines. This talk will give an overview of what HPC is, who uses it and why.

SIMPSON, Alan D (EPCC, The University of Edinburgh, UK)

HPC architectures

HPC architectures form the cutting edge of modern computer technology and is an area of active research, rapid developments and high risk business. This session will review the current state of the art in HPC hardware, from multiprocessor PCs to the world's largest supercomputers, and give an indication of likely future trends in the industry.

BULL, Mark (EPCC, The University of Edinburgh, UK)

Basic Concepts of OpenMP

This session will cover the fundamental concepts of shared memory parallel programming, including threads and thread teams, shared and private memory, dependencies and synchronisation. We will also describe the basic syntactical and semantic structures in OpenMP.

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GRAHAM, Paul (EPCC, The University of Edinburgh, UK)

Parallel Loops

Loops are the principal source of parallelism in many applications. This session will describe the support in OpenMP for parallelising loop constructs, including private variables, reductions and scheduling options.

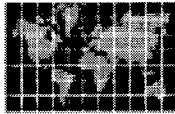
HENTY, David S (EPCC, The University of Edinburgh, UK)

Parallel Regions and Synchronisation

This session will introduce the fundamental construct in OpenMP, the parallel region, giving examples of its use. In addition, we will describe facilities in OpenMP for achieving synchronisation between threads such as barriers, critical sections and atomic updates.

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ABELL, Martha L (Georgia Southern University, USA)

Multiple comparisons for means

Most commonly used multiple comparison procedures for families of population means are categorized as either single-step or stepwise. Single-step procedures include those for all pairwise comparisons, those for many-to-one comparisons, and those for contrasts. Common stepwise procedures do not guarantee that the familywise level of significance is not exceeded for every possible configuration of the population means. Procedures like that of Peritz remedy this problem. In addition to writing common single step multiple comparisons procedures in Mathematica, we take advantage of Mathematica's capabilities to write stepwise procedures including two based on the Peritz procedure.

ABELLO, James (Shannon Laboratory, AT&T Labs-Research, USA)

Navigating graph surfaces

A broad spectrum of massive data sets can be modeled as dynamic weighted multi-digraphs with sizes ranging from tens of gigabytes to petabytes. These data repositories pose interesting visualization and computational challenges. We introduce the notion of *graph surfaces* as a metaphor that allows the integration of computation over these data sets with their visualization. By using out-of-core algorithms we build a hierarchy of graph surfaces that represents a virtual geography for the given data. To provide the user with navigation control and interactive response, we incorporate several geometric techniques from 3D computer graphics like dynamic visibility processing and mesh simplification. We highlight the main algorithmic ideas behind the tools and formulate some novel mathematical problems that have surfaced along the way. This is a joint work with Shankar Krishnan.

ACHE, Gerardo A (Facultad de Ciencias-Universidad Central de Venezuela, Caracas, Venezuela)

Numerical solution of a second-order quasilinear elliptic partial differential equation in certain unbounded cylindrical domains

In this paper we consider a connected and unbounded domain $\Omega \subset R^3$ given by $\Omega = \Omega_1 \cup \Omega_2 \cup \Omega_3$, where Ω_2 is a compact set with smooth boundary, Ω_1 and Ω_3 are semi-infinite cylinders of radio a_1 and a_2 respectively. The purpose of this research is to solve numerically the following quasilinear elliptic partial differential equation: $\Delta u + \lambda f(u) = 0$, $x \in \Omega$ and $u = 0$ for $x \in \partial\Omega$, and the regularity condition, $u \rightarrow U_i^\infty$, for $|x| \rightarrow \infty$ and $x \in \Omega_i$ ($i = 1$ or 3), for a given U_i^∞ . We used a second order finite difference scheme to discretize the partial differential equation and a conjugate gradient type of method, to solve the linear systems resulting from the Newton iterations. We determine an exponential decay estimate for this equation which was used to derive computational boundary conditions, able to reduce the unbounded domain into a bounded one, for computational purposes, in a very efficient way. Finally, we present numerical results, for particular f and λ , to demonstrate the effectiveness of our approach.

ADINTSOVA, Antonina I (Belarus State Economic University, Belarus)

Monotone graphs with threshold survival

Earlier there were given characterizations of complex systems modeled by K-terminal undirected networks having threshold survival. In such networks elements have "destruction costs", and the network is disconnected if and only if its total cost exceeds threshold value. As for directed networks the corresponding problem has remained open. The solution of this problem directly follows from the presented characterization of dc-trival graphs with threshold survival. Dc-trival graphs are the subset of monotone graphs including as special cases classic reliability network models. The general class of monotone graphs is proved to be recognized in time polynomial in the number of minpaths. This is joint work with A A Chernyak.

AKHMETOV, Marat (West Kazakhstan Economical and Financial Institution, Kazakhstan)

The comparison method for vibroimpact mechanisms

We are suggesting a new method of investigation of vibroimpact systems with impulse actions on surfaces. As an example of the application of our results, the problem of existing of a center and a focus of discontinuous dynamical Lyapunov's system on a plane is considered. The set of discontinuity points is nonlinear.

ALAM, Rafikul (Indian Institute of Technology Guwahati, India)

On the approximation of stable invariant subspaces

Invariant subspaces of bounded linear operators play an important role in many applications. The fact that invariant subspaces are very sensitive to perturbation makes it difficult to approximate. It is well known that spectral subspaces, that is, maximal invariant subspaces are relatively well behaved in the sense that under suitable hypotheses these subspaces can be approximated. Error bounds are available for the approximation of maximal invariant subspaces under various notions of convergence. The purpose of the present paper is to show that stable invariant subspaces which are not necessarily maximal are stable under small perturbation. We obtain error estimates for the approximation of stable invariant subspaces under a mild hypothesis on the approximating operators. Let T be a bounded linear operator on a Banach space X . Suppose that $Y \subset X$ is a stable invariant subspace of T . If T_n is a sequence of bounded operators on X which approximates T in some sense then, among other things, we show that there is a stable invariant subspace $Y_n \subset X$ of T_n such that $\theta_s(Y, Y_n) \leq \text{constant} \times \|(T - T_n)T\|$ for all large n , where $\theta_s(Y, Y_n)$ is the spherical gap between Y and Y_n .

ALDUNCIN, Gonzalo (Institute of Geophysics, UNAM, Mexico)

Macro-hybrid mixed finite element schemes for control advection-diffusion problems

The purpose of this paper is to present Uzawa and penalty-duality algorithms for macro-hybrid mixed finite element models of evolution control advection-diffusion problems. The central idea is to introduce nonoverlapping domain decompositions, with transmission conditions across the internal boundaries modelled and dualized subdifferentially. Then, finite discretizations are introduced, in general, globally nonconforming and of a nonmatching grid nature. An abstract presentation of this theory has been given in Numer. Funct. Anal. & Optimiz. 19 (1998) 667-696. Finally, computational experiments are presented comparing the diverse algorithms, and analyzing the optimal parameters.

ALEKSANDROVA, Svetlana (Coventry University, UK)

Buoyant convection in a rectangular box with horizontal temperature gradient and strong vertical magnetic field

Three-dimensional buoyant convection in a rectangular cavity with horizontal temperature gradient in a strong, vertical magnetic field is considered. An asymptotic solution of the problem in the inertialess approximation is obtained for high values of the Hartmann number, Ha . The three-dimensional flow is characterized by the presence of high-velocity jets at the vertical walls of the cavity. The velocity of the jets is $O(Ha)$ time higher than in the bulk of the fluid. This makes the flow qualitatively different from its two-dimensional counterpart, studied before. Concerning Bridgman crystal growth applications, the results have serious implications for mass transfer.

ANDERSON, Harry C W (AMAC, Cranfield University, UK)

Quasi-steady state model of a gravity driven fluid sheet

The motion of thin liquid films is of fundamental importance in many industrial applications, ranging from surface coating to heat exchanger design. The following investigation has a particular application in the formation of runback water films on aircraft during flight, and stems from analysis of an experiment to understand this problem. The experimental setup was constructed to mimic the motion of a film down an inclined plane, or 'draining flow'. In this presentation, a brief description of the experiment is given, followed by a discussion of the derivation and analysis of a quasi-steady state model of the observed motion. The model is derived from the standard lubrication approximation to the Navier-Stokes equations. It considers the flow as three separate regions; inlet, intermediate and leading edge. A perturbation of the equilibrium solution in the intermediate region is obtained to provide initial values for the solutions at the inlet and leading edge. These solutions are then marched forward to provide a film shape over the whole region. The presentation will conclude with a comparison of the results with an alternative finite element solution developed at Cranfield. Sponsored by British Aerospace, Sowerby Research Centre, Filton.

ANGULO, Oscar (Universidad de Valladolid, Spain)

A characteristic method for nonlinear size-structured population equations

Size is one of the most natural and important physiological attributes for the individuals of populations in many species, typical examples are fishes and trees. Structured population models reflect the effect of the physiological state of the individuals on the population dynamics. In addition, nonlinear structured population models allow to take into account the effect of the total population in the structured-specific growth, mortality and fertility rates.

We consider the numerical integration of the nonlinear size-structured population model, which is an extension of the model proposed by Murphy. We introduce an explicit method of characteristics and show its efficiency applied to several examples.

ANTIMIROV, Maximilian Ya (Riga Technical University, Latvia)

Analytical solutions for the problems of the flowing into of the conducting fluid through the lateral side of the plane channel in a strong magnetic field

The exact analytical solutions are obtained in cases when fluid flows into through a split with bounded width or through a round hole. An external uniform magnetic field is parallel or perpendicular to the lateral side of the channel. The Stokes and inductionless approximations are used (magnetic Reynolds number $Re_m \ll 1$). From exact solutions the asymptotic expressions of velocity and pressure of the fluid are obtained for big Hartmann numbers Ha . These results can be used in calculations of cooling systems for projectable thermonuclear reactors. This is joint work with E S Kozlova.

ANTIPOV, Yuriy A (University of Bath, UK)

Exact formulae for the weight functions of the 3-d-problem of an interfacial semi-infinite plane crack

The problem of a semi-infinite plane interfacial crack between three-dimensional isotropic half-spaces is considered. Mathematically the problem is reduced to the analysis of the 3×3 matrix Wiener-Hopf problem. The task of splitting the Wiener-Hopf kernel into two parts is achieved in terms of matrices which are analytic in the upper and lower half-planes, respectively, except at a finite number of poles. The subsequent elimination of these singularities leads to the exact solution of the problem in quadratures. The explicit expressions for the stresses, discontinuities of the displacements, the stress intensity factors and the weight functions are constructed. The formulae for the weight functions are expressed through improper integrals with an exponent-law decrease of the integrands. In a special non-homogeneous case of the elastic constants of the half-spaces the weight functions are found in elementary functions. By passing on the limit $\lambda \rightarrow 0$, where λ is a parameter of the Fourier transform, a solution of the 2-D-problem is obtained.

ANTOINE, Marie-Joelle (Laboratoire CERMA, France)

A proposal for the numerical simulation of urban microclimates

We present a program to calculate the surface temperatures of any urban site, modelled as a set of polygonal facets of known thermal properties. The urban site is submitted to local climatic conditions (sunlighting, wind and sky vault action). We treat radiative exchanges using adapted versions of the progressive refinement radiosity algorithm, as well as conductive and convective transfer.

At the present time, we are working on a sensitivity study for this program, and on an extension to include vegetation effects (partial shading and evapotranspiration). This application can be used to assess environmental properties and comfort levels of urban forms.

AOYAMA, Yuji (Toyo Communication Equipment Co Ltd, Japan)

Component mode synthesis for large scale structural vibration analysis

We propose new combination of the mode to be used in the component mode synthesis. It is to be shown that the proposed method is more adequate for extremely large scale vibration analysis than the conventional component mode synthesis. The proposed method has features as (1) Computation cost is low. (2) Memory size is small. (3) Exactness of the solution is fine. By implementing a system to which the method is applied, analysis of a scale of ten million degrees of freedom was performed. This is a joint work with G Yagawa and K Hiramata.

ARBENZ, Peter (ETH Zürich, Institut für Wissenschaftliches Rechnen, Switzerland)

A comparison of Eigenvalue solvers for electromagnetic fields in cavities

We investigate algorithms for computing steady state electromagnetic waves in 3D cavities. The Maxwell equations for the strength of the electric field are solved by (1) a penalty method using quadratic finite Lagrange elements, and (2) a mixed method with quadratic Nédélec elements. Both approaches avoid spurious modes.

The resulting large sparse matrix eigenvalue problems are solved (1) by implicitly restarted Lanczos algorithm and (2) by Jacobi-Davidson algorithm. The systems of equations occurring in each iteration step are solved by the conjugate gradient method combined with a two-level hierarchical basis preconditioner. We compare the amount of work it takes each solver to compute a few eigenpairs to a given accuracy.

ARIPOV, Mirsaid (Tashkent State University, Tashkent, Uzbekistan)

One splitting method for some class of the quasilinear equations

The method of nonlinear splitting for some class of the quasilinear parabolic, hyperbolic and elliptic type of equations and their system, which are the basis for modeling various nonlinear processes is offered. This method allows to reduce multidimensional nonlinear equations in particular derivatives to self-similar or approximately self-similar forms. In parabolic case based on the obtained equations and comparison theorem different properties weak solution of Cauchy problem, in particular asymptotics of fronts and solutions of a near the front, that agree with physical process are established. The numerical calculations are carried out by using the estimates for the solutions.

ARKIN, Vadim I (Central Economics and Mathematics Institute, Russia)

Investment under stochastic environment

Authors propose a model of investment in new projects which profits are described by stochastic process. The profit of the investor depends on the parameters of both the project, and economic environment (prices, discount rates, and tax system). A specific feature of the model is a possibility to delay the decision to invest the project before obtaining new information on the environment. The purpose of the investor is to find such a moment for investment that his expected discounted net income will be maximal. We obtain explicit formula for the optimal investment moment and use it for the analysis of the dependence of the indicators of investment activity as well as some accompanying indicators on the parameters of uncertainty, risk, and tax policy. The results are based on optimal stopping theory for stochastic processes, but unlike the traditional heuristic "smooth pasting" arguments we propose straightforward and rigorous approach to finding the optimal stopping time (investment moment).

ARULIAH, Dhavide A (University of British Columbia, Canada)

A method for the forward modelling of 3D electromagnetic quasi-static problems

We present a solution method for solving electromagnetic problems in three dimensions in parameter regimes where the quasi-static approximation applies and the permeability is constant. By using a potential formulation with a Coulomb gauge, we circumvent the ill-posed problem in regions of vanishing conductivity, obtaining a system of elliptic, weakly coupled partial differential equations. The strongly elliptic system thus derived leads to a robust finite-volume discretization. We solve the resulting large, sparse algebraic systems using preconditioned Krylov space methods and demonstrate the efficacy of our method in several numerical experiments.

ARUN, C P (Department of Urology, Ayr Hospital, Ayr, UK)

Queueing theory in clinical practice: Application to the gastro-intestinal system

Queueing theory or Congestion theory deals with probabilistic models of systems where service is required by a customer who waits in a queue if he cannot be served immediately. In biology, queueing theory has been employed in models in theoretical and experimental psychology, epidemiology, drug pharmacokinetics and animal physiology. In a previous paper, we introduced a queueing theory based model of the lower urinary tract (See CP Arun(1998): *Queueing theory in clinical practice: application to the lower urinary tract*. Paper presented at the IMA Conference on Mathematical Applications in Medicine and Biology, Oxford, England). In the present paper, we present a model of the gastro-intestinal system based on queueing theory. Quantitative simulation was performed using discrete event simulation software.

The gastro-intestinal system may be viewed from a queueing theory standpoint as comprising a series of servers in series. The stomach, small and large bowel and rectum may be obstructed, leading to congestion of the system. On the other hand, rapid transit could lead to diarrhoea and malnutrition. Food and water enter the body through the mouth. Food undergoes digestion and absorption from the gastro-intestinal tract (GIT). The process of digestion requires the mediation of digestive juices from the stomach, the pancreas, liver and gall bladder and intestine. Out of about 1500 ml. of food, and about 6500 ml. of intestinal and other secretions, only 200-300 grams is lost as faeces. Functional or organic obstruction of a viscus leads to distension of the GIT proximal to the site of obstruction. To help repair the server, clinically one employs stoppage of oral intake, nasogastric suction to relieve the congestion. In cases of functional obstruction, this alone may suffice. In the event of organic obstruction of course, surgical relief may be required. This model provides a fresh perspective on GIT dysfunction in the light of queueing theory.

ASCH, Mark (Analyse Numérique et EDP, Université Paris-Sud, France)

Exact controllability of wave equations on complex geometries using a composite grid method

A composite grid finite difference (CGFD) method is used to study exact controllability of the wave equation and of the linear elasticity system. On complex geometries, waves can be trapped in sub domains. By localising these domains numerically, we obtain information concerning the optimal placement of captors and sensors for the control of the underlying system. We present numerical results of large-scale simulations and introduce an energetic cost factor (ECF) that effectively indicates the presence of trapped rays.

ASSATOUROVA, Julia (St Petersburg State Technical University, St Petersburg, Russia)

Financial models for decision making in trading business

The paper is devoted to the development of mathematical models for financial stream simulation in trading business. The original algorithm for the model development is presented. On the base of the algorithm particular financial models are developed. These models vary in the investment principles. Utilisation of the obtained models for decision making in trading business is shown. The models give businessmen the opportunity to provide fast, necessary calculations in order to make decisions. Decision making principles in conditions of risk and indeterminacy are considered. In particular, the solution of the problem of working capital calculation and optimisation is shown.

ATKINSON, Kendall E (University of Iowa, Iowa City, Iowa, USA)

The planar radiosity equation and its numerical solution

The radiosity equation is an integral equation arising in both the study of global illumination models and radiative heat transfer. This talk discusses properties of the planar radiosity equation and methods for its numerical solution. Regularity properties of the radiosity solution are summarized including both the effects of corners and the effects of the visibility function. These are taken into account in the design of collocation methods with piecewise polynomial approximating functions. Some numerical examples conclude the talk.

AUCHMUTY, Giles (Department of Mathematics, University of Houston, USA)

The 3D magnetostatic boundary value problem

Variational principles for magnetostatic equilibria under given body and surface currents are described. Necessary and sufficient conditions for the existence of unique finite energy solutions are described. These require certain fluxes be prescribed if the domain has non-trivial differential topology. Some features of the solutions of these well-posed problems will be developed.

AVRACHENKOV, Konstantin (University of South Australia, Australia)

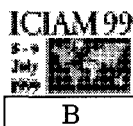
Perturbation analysis of reduced resolvents and generalized inverses

We investigate analytic perturbations of the reduced resolvent of a finite-dimensional linear operator (also known as Drazin inverse in the linear algebra literature). Our approach is based on spectral theory of linear operators as well as on a new notion of group reduced resolvent. It allows to treat regular and singular perturbations in a unified framework. We provide an algorithm for computing the coefficients of the Laurent series of the perturbed reduced resolvent. In particular, the regular part coefficients can be calculated by simple recursive formulae. Finally, we apply these results to the perturbation analysis of Moore-Penrose generalized inverses. This is a joint work with Jean B Lasserre.

AWBI, Bassam (University of Perpignan, France)

Dual formulation of a quasistatic viscoelastic contact problem with Tresca's friction law

We consider quasistatic evolution of a viscoelastic body which is in bilateral frictional contact with a rigid foundation. We derive two variational formulations for the problem: the primal formulation in terms of the displacements and the dual formulation in terms of the stress field. We prove the existence of a unique solution to each one and establish the equivalence between the two variational formulations. We also prove the continuous dependence of the solution on the friction yield limit.



BALASHEVICH, Natalia V (Institute of Mathematics, National Academy of Sciences, Belarus)

Construction of bounded stabilizing feedbacks for dynamical systems

The stabilization problem for continuous dynamical systems is considered. A method of synthesis of bounded stabilizing feedbacks is proposed. The main idea of the method consists in introducing special optimal control problems and in realizing their positional solutions in real time. It is proved that the optimal feedback for an auxiliary optimal control problem is a bounded stabilizing feedback for the dynamical systems to be stabilized. Choice of the control criterion of an optimal control problem influences the quality of a transient. Algorithms of operating three types of stabilizers based on three types of optimal control problems are described.

BARONE, Piero (Istituto per le Applicazioni del Calcolo, CNR, Italy)

The numerical inversion of the Laplace transform to solve the nuclear magnetic resonance relaxometry problem

The NMR relaxometry problem can be formulated as a noisy constrained moment problem with respect to the exponential basis. Its solution requires therefore the numerical inversion of the Laplace transform of the non negative target function in a specific interval of \mathbb{R}^+ . Many general methods are available to solve this problem both in a continuous and discrete frameworks. However all of them have some drawbacks and limitations. We develop therefore new methods which possibly take into account the specificity of the relaxometry problem. In order to overcome the ill-posedness of the problem, implicit and explicit regularization procedures are considered both in a deterministic and stochastic frameworks. We also consider the combination of more than one method for further improving the final result.

BARTON, Stanislav (Dept. of Physics, Mendel University in Brno)

LSQ method for nonlinear piecewise defined functions - Maple solution

The aim of the work is mathematical formulation of fast algorithm of computation of coefficients of two piecewise defined nonlinear functions. The pattern of grow of animals can be used as an example. Let us assume new form of pattern of grow in form of two different exponential functions, applicable in definite interval only. Thus, $F_1(t) = a_1 + b_1 e^{t/c_1}$ for $-\infty \leq t \leq \xi$ and $F_2(t) = a_2 - b_2 e^{-t/c_2}$ for $\xi \leq t \leq \infty$. The first function is describing the increasing weight of animal, starting at natal weight. The second function is describing decrease of weight grow until the constant weight of adult animal. The functions are piecewise defined and including general time interval change of function validity ξ , contain 7 free coefficients, 3 of them non-linear. Two linear coefficients are given by conditions of continuity. The rest of coefficients 2 linear and 3 non-linear c_1 , c_2 and ξ is determined by combination of least square method and Newton's iterative method. Considering the high mathematical difficulty of given problem, the solution of algorithm is derived in symbolic algebra programme MapleV.5.1.

BARUCQ, Hélène (Université de Pau et des Pays de l'Adour, Pau, France)

Outflow boundary conditions for first-order pseudo-differential systems

This work deals with a general approach for the construction of outflow boundary conditions for first-order strictly hyperbolic pseudodifferential systems. It is based upon a recursive and algorithmic formulation of Taylor's diagonalization procedure. Conditions are of arbitrary order and can be applied on the surface of arbitrary regular shaped domains. An example of application is given for Maxwell's system in Transverse Electric polarization. New radiation boundary conditions are designed and numerical experiments show their efficiency for the computation of the scattered field. This is a joint work with X Antoine.

BATISCHEV, Vladimir Andreevich (Rostov State University, Russia)

Bifurcations of stationary regimes of fluid flow in viscous layers

The problem of bifurcations of self-similar solutions for the stationary fluid flow in horizontal layers are investigated when the temperature gradient influences at the free surface. Supposing axial symmetry and absence of peripheral component of velocity there are constructed self-similar solutions for Boussinesk-Oberbeck equations. For these solutions the dependencies of pressure gradient from layer thickness are derived numerically and analitically. The branching problem for the obtained solutions is studing by the well-known method. At each point of branching there appear a pair of new simetric self-similar solutions differing from the previous by presence of rotation around the symmetry axis. Outside the vicinity of bifurcation points the branching solutions are obtained numerically and asymptotically.

BAUMANN, Helge (University of Hamburg, Germany)

Aeroassisted orbit transfer with finite thrust

We consider a coplanar Aeroassisted Orbit Transfer (AOT) from a circular high earth orbit to a circular low Earth orbit with the purpose of minimizing the fuel consumption. Starting from a model with the assumption of two impulses of thrust the equations of the adjoint variables and the nonlinear control, i.e. the lift parameter, are formulated. This model is evolved to a new one with two phases of finite thrust and two new controls, i.e. the magnitude and angle of thrust. Now the complete trajectory can be optimized, instead of the atmospheric part only. Numerical results satisfying the first order and second order necessary conditions are presented. This is a joint work with H J Oberle.

BAUMGART, Andreas (Forskningscenter Risø, Prøvestationen for vindmøller, Denmark)

Aerodynamic stability of wind turbine blades

Self-excited oscillations of wind turbines are thought to result from interaction of flexible blades and airflow. A mathematical model is presented for one blade and the airflow around the blade. The blade rotates around a fixed horizontal axis which is perpendicular to the longitudinal blade axis. It is modelled as a rod accounting for flexure, torsion, stretching and warping. For the flow, a phenomenological dynamic stall model is chosen. It consists of few nonlinear differential equations describing basic flow characteristics. Its state variables are related to aerodynamic loads on the blade. Blade and airflow are discretized using Finite Elements. Conditions for self-excitation are given as a result of linear stability analysis.

BÉDA, Peter B (HAS-TUB Research Group of Dynamics of Machines and Vehicles, Technical University Budapest, Hungary)

Dynamical systems in modelling of material instabilities

Material instability phenomena (strain localization or flutter) are of great importance in solid mechanics. They could play an essential role in catastrophic damage of structures or machines. The classical studies of them investigate the eigenvalues of the so-called acoustic tensor describing the possible wave-speeds in the material.

In this paper dynamical systems theory is applied to perform linear and non-linear stability and bifurcation investigations. By using the basic equations of solid continua an equation of motion is obtained and material stability is treated as Lyapunov stability of some special solution of the dynamical system defined by the equation of motion.

BELEN, Selma (University of Adelaide, Adelaide, Australia)

Stochastic rumours with general initial conditions

The analysis of stochastic rumours generally assumes a fixed finite number (often unity) of spreaders and no stiflers. For some applications this is inappropriate. In this paper, we address the Maki-Thompson rumour model in which arbitrary proportions of the initial population are spreaders and stiflers. We show that as the population size tends to infinity with fixed initial proportions of spreaders and stiflers, the final proportion of ignorants tends to a limit depending on those initial proportions. We also discuss some computational aspects by using our computer simulation results. This is a joint work with Assoc. Prof. C E M Pearce.

BERGLEZ, Peter (Department of Mathematics, Graz University of Technology, Austria)

On the solution of a generalized Stokes-Beltrami system

In this lecture a generalized Stokes-Beltrami system of the form $a(z, \bar{z})w_z = w_z^*$, $b(z, \bar{z})w_{\bar{z}} = w_{\bar{z}}^*$ is considered where a and b denote matrix valued functions and w and w^* are vectors. Using special differential operators we discuss several properties of the solutions. For particular coefficients a and b we give general representation theorems for the solution in simply connected domains as well as in the neighbourhood of isolated singularities.

BICA, Ion (Schulmberger-Doll Research, USA)

Schwarz analysis of iterative substructuring algorithms for the p -version finite element method

Iterative substructuring methods for linear elliptic and parabolic problems, discretized by the p -version finite element method are considered. The objective is to design algorithms in 3D for which the convergence rate grows slowly with the maximum degree p of the polynomials in our finite element space.

The main challenge was how to use and further develop extension theorems for polynomials in order to explicitly construct the basis functions and, consequently, obtain bounds on the convergence rate of several algorithms. Similar work for the h -version and spectral finite elements has been done by several authors, but our case poses new challenges.

BISCAIA, Evaristo C, Jr (COPPE/UFRJ, Rio de Janeiro, Brazil)

Solving large scale DAE models in PVP platforms

The rigorous model of a multitubular catalytic reactor, a large-scale DAE system comprising about 200,000 equations, was integrated through BDF technique. Solution for the resulting set of sparse, non-symmetric, linearized equations is accomplished with a specially tailored preconditioned GMRES iterative driver. This technique, when considered within the framework of an element-by-element (EBE) approach for the overall data structure, provides a natural way to handle the sparsity of the global jacobian which is actually never assembled. Good vector and parallel performance were observed in the test runs carried out on a shared memory, parallel-vector-processor (PVP) platform (CrayJ90). The outcome from the use of more realistic reactor models, made computationally feasible under the approach reported herein, is the driving force for the continuing research efforts in this area at COPPE/UFRJ. This is a joint work with R.Chasse, J.Alves and A.Coutinho.

BODNÁR, Tomáš (Czech Technical University, Prague, Czech Republic)

Numerical simulation of flow and pollution dispersion in 3d atmospheric boundary layer

The vast time-scales of changes in Atmospheric Boundary Layer require large time-steps for numerical solution, which is in strong contradiction with stability conditions of explicit schemes for high Reynolds numbers. On the other hand fully implicit schemes are relatively complicated and expensive. The numerical model proposed in this paper offers a new fast alternative approach to the solution of the boundary layer approximation, together with pollution dispersion on simple geometries. The system of governing equations is solved using semiimplicit scheme based on finite difference discretisation on structured body-fitted mesh. The simple algebraic turbulence closure was used. This is a joint work with K Kozel, P Fraunié and Z Jaňour.

BOOKER, Stuart M (Department of Mathematics, University of Dundee, UK)

Effective disruption of nonlinear electronic sub-systems

We consider the disruption of nonlinear electronic sub-systems by periodic waveforms. These circuits cannot simply be characterised by their spectral response to sinusoidal excitations. In consequence, the threshold for chaotic dynamics (or for bifurcation into multiperiodic behaviour) is strongly waveform dependent. We illustrate this dependence for the phase-locked loop and the automatic gain control loop, and discuss how to design an optimal waveform for disrupting such sub-systems. An analysis based on Melnikov's method is supported by direct numerical solution of the dynamical equation. Comparison is made with available experimental evidence.

This is a joint work with Paul D Smith, Department of Mathematics, University of Dundee, UK.

BOSSAVIT, Alain (Électricité de France)

Yee scheme, FDTD, Whitney forms: A new synthesis

Yee's scheme, also known as the "finite differences in time domain" (FDTD) method, solves transient Maxwell equations in explicit leapfrog fashion. With finite elements (Whitney forms), the analogous approach requires diagonal lumping of mass matrices, for which good rationales are not easy to find. On the other hand, so-called "finite integration techniques" seem to bypass this difficulty and even, to avoid any recourse to finite elements, while still allowing nonuniform grids. From a new viewpoint (focusing on the discretization of the Hodge operator of differential geometry), we attempt a synthesis between these two schools of thought.

BOTCHEV, Mike A (CWI, The Netherlands)

A zoom technique for advection schemes in air pollution modelling

Regional space-grid refinement (zooming) is desirable in many applications, e.g. in Air Pollution Modelling (APM). Typically, in APM advection is integrated in time explicitly, so that the CFL step-size restriction is most severe in the zoom region. If the most refined part of the grid contains few cells, using the same timestep τ everywhere is inefficient because τ is then unnecessarily small for the relatively many remaining cells. On the other hand, allowing different step sizes in regions with different resolutions creates additional overhead and raises questions about mass conservation, positivity, etc. at the zoom-region boundaries. We present an algorithm that meets the relevant requirements while preserving efficiency and parallelism as much as possible.

This is a joint work with P J F Berkvens, W M Lioen, J G Verwer.

BRAAMS, Bastiaan J (Courant Institute, NYU, USA)

Electronic structure calculations via semidefinite optimization

The one-body and two-body reduced density matrices are the fundamental objects of study for electronic structure calculations in an approach that reduces the ground state eigenvalue problem to a linear optimization problem subject to representability conditions that comprise linear equalities and bounds on eigenvalues. We are re-investigating the theoretical power of this approach, including some new representability conditions, and are studying the effectiveness of newly developed interior-point and subgradient bundle methods for the resulting large semidefinite optimization problem. This is joint work with Shidong Jiang, Madhu Nayakkankuppam, François Oustry, Michael L. Overton and Jerome K. Percus.

BRAUN, Richard J (University of Delaware, USA)

Insoluble surfactant model for draining film with surface viscosity

The evolution of the deforming free surface of a vertically-oriented thin film draining under gravity is examined for the case where there is an insoluble surfactant with finite surface viscosity. The surface is assumed to have Newtonian properties. Three coupled nonlinear partial differential equations describing the free surface shape, a component of the vertical velocity and surfactant transport are obtained at leading order without inertial effects. Interfacial stresses resulting from finite surface viscosity and Marangoni effects are included. We first examine the case where the film is sufficiently flat so that mean surface tension is negligible, this will result in tight bounds on the limits of experimental data obtained at Dow Corning. Various other cases will be described as time permits. This is a joint work with S Naire, University of Delaware and S A Snow, Dow Corning.

BRAUN, Richard J (University of Delaware, USA)

Two phase viscous drop spreading

The spreading of a thin drop under a thin film is studied using lubrication theory for both phases. The resulting pair of evolution equations for the free surfaces of the film and the drop are studied using both pseudospectral and finite difference methods. The results for the case of a perfectly wetting drop covered by a perfectly wetting film is considered first. Results for a drop that partially wets the substrate will be presented if available.

BRÉE, David S (University of Manchester, UK)

Most-perfect magic squares

We have developed a method for constructing and enumerating all squares of any size in an interesting class of magic squares, which we call 'most-perfect'. This is the first time, in the thousand years during which magic squares have challenged mathematicians, that a method of construction, let alone enumeration, has been found for a whole class of magic square. In most-perfect squares integers come in complementary pairs along the diagonals and any 2×2 block of four adjacent integers add to the same sum. These properties ensure that most-perfect squares are pandiagonal magic squares. A method of constructing and a formula enumerating all most-perfect squares are given. There is a remarkably large number of these squares. This is a joint work with Dame Kathleen Ollerenshaw.

BROADBRIDGE, Philip (University of Wollongong, Australia)

Symmetry analysis of equations of solute transport in soil

Solute transport in saturated soil is described by a Fokker-Planck equation coupled to Laplace's equation for the water velocity potential. Lie symmetry techniques are used to find new similarity solutions in 2+1 dimensions, when the water velocity field is more complicated than the uniform, point-source or corner-flow fields that have been treated previously. Extra complications that must be considered, include the dependence of solute dispersion coefficient on the water velocity, and non-uniform water concentration in unsaturated soil.

BRYKALOV, Sergei A (Institute of Mathematics & Mechanics, Ekaterinburg, Russia)

Systems with nonlinear nonlocal boundary conditions

The solvability and some qualitative properties are studied for problems with nonlinear functional boundary conditions for ordinary differential and functional differential equations. Monotonicity assumptions on boundary conditions are obtained that together with some other natural restrictions ensure the solvability. Boundary conditions of similar type arise in control theory. In particular, they arise in connection with steady-state temperature distributions in some feedback heating control systems with movable point sources. They arise also in connection with the choice of terminal moment of a differential game by one of the players with the help of a continuous mapping. Supported by RFBR, 97-01-00160.

BUELLESBACH, Juergen (Universitaet der Bundeswehr Muenchen, Germany)

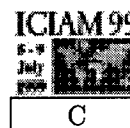
On the influence of geometrical imperfections on stability behaviour of shell constructions

In literature, the usual way to consider the influence of imperfections on the stability behaviour of elastic shells is to re-modell the (imperfect) geometry of the construction - e.g. by using Finite Elements - and to calculate the stability of this (new) structure. Nevertheless, this procedure has some remarkable disadvantages: The most important one is that for every new shape of imperfection, the geometry has to be re-modelled and the considered fundamental state has to be re-calculated - an enormously ineffective (numerical) working method. Furthermore, this way of considering an imperfection does not fit with the usual idea of an imperfection namely as disturbance of a perfect initial state. Taking into account these disadvantages, a method to estimate the stability behaviour of shells using only the initial state and the fundamental state of the perfect shell is presented. The results obtained are compared with those to be found in literature and with other examinations which were developed by using the Finite-Element-Program-System MSC/Nastran.

BULIGA, Marius (Institute of Mathematics of the Romanian Academy, Romania)

Energetic criterions in brittle fracture mechanics

Sih's criterion for brittle crack propagation has been experimentally validated in the case of mixed mode I-II crack propagation in isotropic linear elastic materials. We propose a new theory of brittle fracture mechanics based on Mumford-Shah energy functionals. This theory can explain the propagation of an arbitrary-shaped crack in a tri-dimensional elastic body. The numerical results obtained with our theory agree with the experimental data which validate Sih's criterion. This match indicates a strong connection between Sih's criterion and our model. This is a joint work with Marius Craciun, Ovidius University, Romania.



CABALLERO-GIL, Pino (University of La Laguna, Spain)

Algorithm-independent attacks on unkeyed hash functions and digital signature schemes

The security of unkeyed hash functions and some digital signature schemes is considered. Various general attack strategies are discussed and exact success probabilities in some of these algorithm-independent attacks are calculated and analysed. In particular, attacks based on a set of known used signatures are studied and classified into "with replacement" and "without replacement", and in both cases, different expressions for success probabilities are obtained. From their analysis, some hints to design optimal strategies for forgers and to choose convenient parameters for the schemes are pointed out. This is a joint work with M I Dorta-González.

CAI, Xiao-Chuan (Department of Computer Science, University of Colorado at Boulder, Boulder, USA)

Simulating 3D compressible flows by coupling multiple models

The development of a multi-model formulation to simulate 3D compressible flows on parallel computers is presented. The goal is to reduce the total simulation time by using a more computationally efficient physical model where possible. This involves splitting the computational domain into different flow regions and using the full potential model instead of the Euler or N.-S. equations in certain regions. In the talk we discuss the full potential and the Euler coupling and the discretization of the interface conditions on fully unstructured 3D meshes. Numerical simulations of transonic flows are presented. This is a joint work with M Paraschivoiu and M Sarkis.

CALDWELL, James (City University of Hong Kong, Hong Kong, China)

Spherical solidification by enthalpy method and heat balance integral method

Phase change problems occur naturally in many physical and industrial processes. These problems possess a moving boundary for which a flux condition expressing the conservation of heat and release of latent heat is satisfied. There are two main approaches to the solution of Stefan problems. One is the front tracking method, which explicitly tracks the phase front and the condition on the moving boundary is enforced. The Heat Balance Integral Method (HBIM), to be used in this presentation, is one such example. Another approach is to use a fixed domain formulation, eg. enthalpy method. There are different ways of tracking the boundary using the enthalpy method. In this presentation, the method is generalized to a spherical geometry and is compared to the result obtained from the HBIM.

CAMARGO-BRUNETTO, M Angelica De O (State University of Londrina, Brazil)

An algebraic algorithm for counting polynomial zeros in a circle using principle of argument and Chebyshev polynomials

An algebraic algorithm for counting polynomial zeros lying in a circle is proposed. It is based on Principle of argument, Cauchy indices and a theorem due to Schelin, where the zeros inside the unit circle is given by $N = I_{-1}^1 p_1/p_0$ ($p_0(x) = \sum a_k T_k(x)$), $p_1(x) = \sum a_k U_{k-1}(x)$), being T and U Chebyshev polynomials. Cauchy Indices can be computed using Sturm sequences and unlike most of polynomials have their coefficients length decrease, which is an interesting property for algebraic approach. Experimental tests were made for different kinds of polynomials, revealing a good performance of the algorithm, comparing it with a modified version of the Schur-Cohn method.

CAPUTO, Barbara (Universita' la Sapienza, Caspur, Italy)

Morphological analysis of mammographic images with Gabor transform and neural network

In this paper we treat the problem of biomedical image understanding, focusing our attention on a special breast cancer pathology, microcalcifications, whose appears in two different shapes: singles or clustered. There are many studies which connect morphology to breast benignant or malignant but all qualitatives. We choose Gabor transform as feature extractor and the output was given as input to a neural network. Network was trained to detect presence or absence of microcalcifications and subsequently was trained to divide the two morphological classes. The methodology proposed gives good results in terms of detection of presence or absence of microcalcifications and interesting results about morfological analysis of pathologies. This is joint work with G E Gigante and Piero Lanucara.

CARGO, Patricia (CEA-CEA Bruyeres, France)

Numerical resolution of the multidimensional bi-temperature magnetohydrodynamics equations

The numerical resolution of the multidimensional bi-temperature magnetohydrodynamics equations is presented. Thermal non-equilibrium is treated by adding an electronic entropy equation. The complete system is solved by an original Roe-type scheme. In order to handle the magnetic field divergency condition without solving any elliptic system, the Powell system is considered. By using the notion of Godunov-type scheme, a linearized Riemann solver is derived. It strictly takes into account the non-conservative character of the system and it involves the extension of the Roe-matrix notion. In one dimension, the scheme reduces to the Roe scheme we have already developed. A simulation of the solar wind around a comet is presented. This is joint work with S Brassier and G Gallice.

CAVIGLIA, Giacomo (University of Genoa, Italy)

Existence and uniqueness in the reflection-transmission process

The reflection-transmission process of time-harmonic plane waves, at a plane interface between two anisotropic viscoelastic solids, is investigated through the sextic Stroh formalism. The direction of a wave is taken to be that of the time-averaged energy flux. Sufficient conditions are determined for existence and uniqueness of the solution to the reflection-transmission problem. The occurrence of surface or interface waves is related to either incompatibility or non-uniqueness of the solution. The phenomenon of the Brewster angle is also pointed out.

This is a joint work with A Morro.

CEPITIS, Janis (Institute of Mathematics of Latvian Academy of Sciences and University of Latvia, Latvia)

Moisture diffusion and attachment in wood

The temperature dependent mathematical model of moisture diffusion and attachment in wood qualitatively and numerically is investigated. There are treatment of wood as a porous medium offered and moisture mass concentration in wood cavities as well as the sorbed cell-wall moisture mass concentration are considered. The obtained results are compared with the experimental practice. This is joint work with Andris Buikis, Harijs Kalis and Andrejs Reinfelds.

CHANG, Chien-Cheng (Institute of Applied Mechanics, National Taiwan University, Taipei, Taiwan)
Numerical study of flow about a finite body by a three-dimensional hybrid vortex method

In this talk, we present a hybrid vortex method for 3-d viscous flow about a finite body. The main features of the method consist of, at each time step, solving the viscous vorticity equation by evolving a total vorticity for each vortex element, and then redistributing the evolved vorticity back to the grid. The (updated) total vorticity on the grid lends itself to accurate reconstruction of the local vorticity field. The velocity is recovered from a Poisson equation for a vector stream function. It is shown consistently to choose the gauge that specifies 0 value for the third component of the stream function. Vorticity is then updated on the solid boundary to fulfill the no-slip condition. Numerical advantages and performance will be illustrated by the model problem of flow about a (rotating) sphere. This is a joint work with CT Wang, National Taiwan University.

CHARPIN, Jean P F (Applied Mathematics and Computing Group, Cranfield University, UK)
Numerical solution for coupled ice growth and water flow

Ice growth may rapidly degrade the aerodynamic performance of an aircraft. Subsequently, de-icing and anti-icing systems have been developed and a number of codes designed to predict the ice shape. When ice accretion starts, two different types of ice can appear, depending on the temperature and conditions. All of the incoming fluid may freeze almost instantaneously and turn into rime ice. Alternatively a part of the incoming fluid may freeze and turn into glaze ice while the other part remains liquid and runs back over the ice. Previous works only focussed on the ice shape and neglected the water layer. The present study takes this thin film into account : it increases the accuracy of the prediction, especially at mild freezing temperatures. The aim of this talk is to describe the numerical solution for the coupled problem of ice growth and water flow on a 2-D flat plane. The first part of the talk deals with the numerical schemes used for this problem. Depending on the type of ice, they are based on a mass balance and an energy balance (glaze ice) or only on a mass balance (rime ice). As both the rime and the glaze ice can form simultaneously, the results give a way of choosing which of the two models is suitable at each point of the surface. The second part of the talk deals with error analysis on these schemes. This study gives relations between the parameters of the discretisation. Finally, future directions will be discussed. This is a joint work with Dr C P Thompson and Dr T G Myers.

CHEREDNICHENKO, Kirill D (Department of Mathematical Sciences, University of Bath)
On derivation of the "higher order" effects in the overall behaviour of heterogeneous media from microstructure

Higher order homogenized equations are derived for an infinite periodic elastic medium with the periodicity cell of size ε , in the presence of a body force f , via a combination of variational and asymptotic techniques. The resulting "higher order homogenized solutions" are rigorously shown to be "best possible" in a certain variational sense, and it is shown that the associated solutions are close to the actual solution up to higher orders of ε . We derive a rigorous full asymptotic expansion for the energy $I(\varepsilon, f)$ and show that its higher-order terms are determined by the higher order homogenized solutions. The resulting variational construction is compared with the "purely" asymptotical one and implications for the choice of the higher order stress-strain relations and for practical implementation are discussed. This is a joint work with V P Smyshlyaev,

CHERNIHA, Natalia D (Institute of Mathematics, Ukrainian Acad. Sci., Ukraine)
Exact solutions of nonlinear boundary value problems with moving boundaries

The mathematical pattern for description of melting and evaporation of metals in the case that their surface is exposed to a powerful flux of energy is considered. In the case of a quasistationary approximation, exact solutions of this nonlinear Stefan-like problem are found. The problem is solved in the (1+1)-dimensional and the (1+3)-dimensional time-space. In both cases the problem for nonlinear partial differential equations is reduced to the ordinary differential equations.

CHERNIHA, Roman M (Institute of Mathematics, Ukrainian Academy of Science, Kyiv, Ukraine)
New exact solutions of non-linear reaction-diffusion equations arising in population dynamics

The method of additional generating conditions (see *Cherniha R Rep.Math.Phys.(1996) vol.38.3, 301; J.Phys.A (1998) vol.31, 8179*) is applied for finding multiparameter families of exact solutions of generalizations of the Fisher equation and a coupled reaction-diffusion system describing spatial segregation of interacting species. The method is based on the consideration of a fixed nonlinear partial differential equation together with an additional generating condition in the form of a linear high-order equation. Some exact solutions are applied for analytical solving the Neumann boundary-value problems of above-mentioned nonlinear equations.

CHERNYAK, Arkadi A (Belarus State University, Belarus)

Universal reliability graph model of cyclic networks

Acyclic monotone graphs admitting arbitrary monotone Boolean functions in their vertices include as special cases all known classes of directed multiterminal network reliability models. Earlier it was introduced the concept of local domination and presented the formula for effective computing domination of acyclic monotone graphs by local dominations of their vertices. In this paper we prove that domination of 0-cyclic monotone graphs is zero. It is given the expression using local domination for computing reliability of arbitrary 0-cyclic monotone graph. The problem of computing domination of r -cyclic monotone graphs is shown to be #P-complete for any integer $r \geq 1$. This is joint work with Z.A. Chernyak.

CHERNYSHENKO, Sergei I (Department of Mathematics, University of Manchester, UK)

Uniqueness of steady flow past a rotating cylinder with suction

The steady two-dimensional incompressible flow past a quickly rotating cylinder with suction is not unique for the velocity at infinity $U_\infty = 0$ and was thought to be not unique also for $U_\infty \neq 0$ since its high- Re asymptotics found by usual methods was not unique. For $U_\infty \neq 0$ the unique asymptotics is determined by an invariant condition derived for arbitrary Re and applied as $Re \rightarrow \infty$. All other solutions obtained by the usual method of matched asymptotic expansions correspond to exponentially small non-zero vorticity at infinity, which cannot be distinguished from zero by this method. This is a joint work with E V Buldakov and A I Ruban.

CHEUNG, C W (Department of Mechanical Engineering and Aeronautics, City University, UK)

An asynchronous algorithm for the solution of unsteady subsonic compressible flow

Many Unsteady aerodynamics codes currently in use in the aircraft industry are still largely based on integral equation methods. Previous work in parallelising these integral equation methods had shown to produce significant savings in CPU times. However, the intrinsic sequential process of matrix coefficient computations and linear system solving cannot be changed. This paper describes an asynchronous algorithm which breaks the intrinsic sequential process. Numerical tests using a network of Sun workstations are included for some unsteady problems. This is joint work with C H Lai.

CHRISTIANSEN, Edmund (Dept. Math.& Comp.Sc., Odense University, Denmark)

Computation of collapse states in limit analysis

A new computational method for the problem of limit analysis with quadratic yield condition is developed and tested. The solution method simultaneously approximates the collapse fields for stresses and flow. Based on these fields a strategy for automatic mesh refinement in limit analysis is developed. The efficiency and accuracy of the approach for large problems is demonstrated by solving a classical problem in the plane strain model: approximately 60000 finite element nodes with 3 stress components and 2 velocity components at each node. In two space dimensions this may be overkill, but it shows that we are able to solve problems in three space dimensions.

CLEARY, Paul W (CSIRO Mathematical and Information Sciences, Australia)

The importance of particle shape in granular flow modelling

Discrete element modelling of granular flows involves following the detailed motions of individual particulate solids and predicting their collisions. Many important industrial applications have been modelled including ball mills and dragline excavators. Traditionally particles are approximated in two dimensions by discs. Such particle assemblies frequently cannot reproduce the behaviour of real materials because the particle shapes are over-idealised. Comparison of DEM simulations using disc and super-quadric particles with experiments demonstrates the importance of shape in four key ways: 1) Effective material strength 2) Dilation during shearing 3) Realistic void distributions 4) Partitioning of energy between linear and rotational modes

CLINT, Maurice (Queen's University of Belfast, N Ireland, UK)

Re-engineering sequential mathematical library software for efficient parallel execution

The effectiveness of high performance computers for the efficient execution of applications software depends critically on the efficiency of the library routines on which the software relies. In this paper the problems faced by software engineers when converting sequential numerical mathematical routines to efficient parallel equivalents are discussed. The re-engineering, for execution on a distributed memory machine, of a number of routines selected from the Harwell Library is described and guidance is offered to those undertaking a similar task. The quality of performance of the parallel implementations is assessed and the algorithmic characteristics which influence their efficiency is commented upon. This is a joint work with K Murphy and R H Perrott, Department of Computer Science, The Queen's University of Belfast, N Ireland, UK.

COLLINS, Derek (University of Sheffield, UK)

Calculating contact pressures from strain and deflection data

In the development of a method for determining experimentally the contact pressures between hard and soft elastic bodies, a beam is loaded by a rubber-faced steel indenter. Deflection and strain are measured along it. The reconstruction of the loading from either set of data is an inverse problem governed by a Fredholm integral equation of the first kind. The deflection problem is more ill-posed than the strain one, but more measurements are available. A projection-type regularization scheme gives reconstructed loadings, which are compared to the loading obtained from a finite-element package. This is a joint work with D A W Taylor and S Quegan.

CONSTANS, Sophie (Cemagref de Bordeaux, France)

Linear formulation for optimizing disinfectant concentrations in water distribution networks

Disinfecting the water supplied by a distribution network directly acts on its quality. Good water quality imposes upper and lower bounds on disinfectant concentrations everywhere in the network, at any time. We propose a linear programming formulation in order to determine the locations where disinfectant must be added and to optimize injection patterns. The objective is to reach target concentration values. The constraints are given by a special code simulating disinfectant propagation and decay under unsteady hydraulic conditions ; they take the system's dynamics implicitly into account. This is a joint work with Bernard Brémond and Paul Morel.

CONSTANTIN, Adrian (University of Zurich, Switzerland)

Wave breaking in shallow water

We present an approach to prove wave breaking for various classes of nonlinear nonlocal shallow water equations.

COOPER, Amanda (University of Ulster at Coleraine, Northern Ireland, UK)

Efficient schemes for external orthogonalization in the Lanczos algorithm

The k -step explicit restart Lanczos algorithms developed by Szularz *et al* for the computation of a few of the extreme eigenpairs of large, usually sparse, symmetric matrices, compute one eigenpair at a time using deflation techniques in which each Lanczos vector generated is orthogonalized against all previously converged eigenvectors. The computation of the inner products associated with this external orthogonalization often creates a bottleneck in parallel distributed memory environments. In this paper methods are proposed which effectively reduce the amount of external orthogonalization required thereby improving the efficiency of the algorithms. The performance of the methods on the CRAY-T3D are assessed. This is a joint work with J Weston and M Szularz, School of Information & Software Engineering, University of Ulster, Coleraine, Northern Ireland. This work was carried out using the facilities of the University of Edinburgh Parallel Computing Centre.

CORTES, Julien (DRN/DEC/SECA CEA Cadarache, France)

Asymptotic analysis of the kinematic disequilibrium for compressible two-fluid flow

This presentation outlines a mathematical method for computing compressible two-fluid flow when the kinematic disequilibrium becomes significant (high interphase relative velocity). In such configurations, the computation of the finite volume method may not be straightforward and stiff source terms may lead to numerical instabilities. Our approach is to first establish an asymptotic model (J. Cortes and al., "A Density Perturbation Method ...", to appear in the Journ. of Comput. Phys.). Such a mathematical approach provides an efficient frame to understand the relevance of interphase convection and relaxation. In conclusion, two-dimensional numerical results, based on Roe-scheme computation, will be presented. This is thesis work done under the direction of Dr I. TOUMI (Saclay).

COUET, Benoit (Schlumberger-Doll Research, Ridgefield, USA)

Distributed optimal control of oil-field reservoirs under uncertainty

Classical stochastic optimal control theory has been developed only for systems with additive noise. We consider the optimal control of systems described by partial differential equations with multiplicative noise. These are equations pertaining to reservoir dynamics. We present a scheme of computing globally optimum stochastic control functions for such systems. Application to multiple-spot oilfield patterns in order to maximise oil-water-cut production rates will be given. Two methods of computing globally optimum control functions will also be given, one deterministic and the other stochastic, and computational comparisons of these two methods will also be presented. This is a joint work with Robert Burrige and Prasana Venkatesh.

COWLEY, Stephen J (University of Cambridge, UK)

Spiral-type vortex breakdown on a trailing vortex: A weakly nonlinear marginal instability?

Experiments demonstrate that there are many routes to vortex breakdown; our concern is with asymmetric, or spiral-type, vortex breakdown. The base flow is taken to be a slowly-varying, high-Reynolds-number trailing vortex. The vortex is assumed to evolve in a downstream axial direction from a stable to an unstable state. Unpublished linear analysis by Yang & Leibovich demonstrates that the swirl is asymptotically large at the point of marginal [in]stability. We derive a modified Landau evolution equation for the amplitude of a weakly nonlinear disturbance, and identify under what circumstances the bifurcation is super- or sub-critical.

This is joint work with M O Souza.

CRACIUN, Eduard M (Ovidius University, Romania)

Fracture of a prestressed isotropic material containing a crack acted by incremental shear stresses

Using the new Sih's fracture theory we determine the direction of crack propagation as well as the critical incremental shear stress assuming the existence of the third fracture mode. Also in the case of a prestressed isotropic material we compare the obtained results with those given by the classical Griffith's and Irwin's theory. Finally we can conclude that the critical incremental shear stress producing crack propagation and predicted by Sih's theory is always smaller as that given by the classical theory. Moreover, according to the new theory the crack will propagate along its line if the initial applied load is a compression and perpendicular to its line if the initial applied load is a traction. This is a joint work with E. Soos.

CRAIK, Alex D D (University of St Andrews, UK)

Second-harmonic resonance with Faraday excitation: Degenerate "bouncing" solutions

The equations $da/dt = -sa + a * -a * b$, $db/dt = -rb + a^2$ describe perfectly-tuned second-harmonic resonance of standing water waves with Faraday excitation. For $r \ll 1$, a virtually complete description of solution trajectories is given. The degenerate case $r = 0$ has a continuum of fixed points. Solutions exhibit "bounces", separated by pauses at unstable fixed points while small random disturbances grow and initiate the next "bounce". Trajectories terminate when a "bounce" reaches a stable fixed point. When $0 < r \ll 1$, a similar structure remains; but all trajectories terminate at one of two available stable fixed points.

CROMME, Ludwig J (BTU Cottbus, Germany)

Process optimization in the packaging industry/energy industry

The production of brown coal briquette bundles in a completely automated production plant imposes strict quality requirements on the pressing of the briquettes. Since briquettes vary statistically in length and weight a quality surveillance must be installed. Such a procedure is presented in this talk, described, and analyzed mathematically. The sensitivity of its parameters turns out to be critical. With this method and other simulation and optimization techniques a dramatic improvement in the overall performance of the plant could be realized. The mathematical fields mainly involved are statistics, analysis, and numerical optimization.

CUMINATO, José Alberto (University of São Paulo, Brazil)

Numerical calculation of unsteady three-dimensional free surface flows in container filling

Due to its practical applications, the motion of fluids with free surfaces has recently, been the subject of much research by engineers and scientists. In this work we describe FREEFLOW an integrated simulation system for three-dimensional free surface flows. It consists of a graphical modelling tool for specifying the domain, initial and boundary conditions using B-Rep data structure, a simulation tool for solving the governing equations and a visualization tool for viewing the results. The results of several experiments designed to investigate the performance of FREEFLOW for different Reynold numbers incompressible flow will be reported. This is a joint work with Valdemir Garcia Ferreira, Antonio Castelo Filho, Murilo F Tomé and Armando O Fortuna.

CUMMINGS, Linda J (Ecole Normale Supérieure, France)

Convection-dominated heat transfer in closed-streamline fluid flows

The problem of heat flow at large Peclet number through a two-dimensional fluid flow (with closed streamlines) is considered. To leading order (in inverse powers of the Peclet number) the streamlines are isotherms, and we derive a one-dimensional diffusion equation for the heat transfer between streamlines. The relevance of the problem to the UHT sterilisation of canned liquid foods is discussed, and in this context we show that the topology of the streamlines within the liquid may have a bearing on the efficiency of the process.

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DAVIDSON, Stuart (Greensboro College, USA)

Uniform heat flow past a circular hole with two symmetrically inclined radial edge cracks

The problem discussed is that of determining the thermal stresses in a linear thermoelastic solid when a uniform heat flow is disturbed by the presence of two symmetrically inclined radial edge cracks. Using a Mellin-type transform and superposition, the problem is reduced to simultaneous singular integral equations. The integral equations are solved numerically and results for the stress intensity factors and crack energy are presented.

DE MAGALHÃES, Maysa S (Department of Industrial Engineering, Pontifícia Universidade Católica do Rio de Janeiro, Brazil)

Adaptive \bar{X} charts - an economic model

Recent studies have shown that control charts with variable parameters detect process shifts faster than fixed parameters control charts. Also, in some industrial systems, it is not convenient to maintain fixed design parameters because of the inherent randomness of the production processes. Then, it is desirable to have a variable parameter policy. We propose an economic model for \bar{X} control charts when all design parameters (sample size, sampling interval, coefficient of control limits) vary in an adaptive (dynamic) way, that is, by using *on-line* information. The hourly cost function is derived. As all parameters vary in an adaptive way, the computation of some of the expected values is non-trivial. Control policy and optimal economic selection of design parameters for \bar{X} adaptive control charts are also addressed. This is joint work with A F B Costa and E K Epprecht.

DE MESTRE, Neville J (Bond University, Australia)

Tournament roulette

Tournament roulette is a game organised by casinos in which players are pitted against each other rather than against the casino. The game is terminated when one of a set of pre-determined numbers comes up after the N th spin, where N may vary across casinos. The object of the game is to accumulate more money at the termination of the game than any other player at the table. The strategies involved in placing bets according to a player's situation at any spin from the N th onwards will be considered.

DE MOURA, Carlos A (DCC/Univ. Fed. Fluminense, Brazil)

Parallel schemes for evolutive differential equations

Despite their load of drawbacks, explicit finite-difference algorithms are largely employed for the numerical solution of evolutive partial differential equations, in particular among communities of application-oriented users, like physicists and meteorologists. For these schemes the constraint CFL-constants impose on the time-step choice may be mitigated, in the case of linear models, with the parallel re-design pattern proposed herein. This inherently load-balanced computing strategy turns out to preserve the scheme stability and accuracy properties, to exhibit a low latency, to allow for time-mesh frequent changes and for easy coupling to space-grid adaptivity tools. Its ideal speed-up - i.e., all communications cost being disregarded - has order $p^3/2^p$, for 2^p active processors. Such an estimate, which points up to massive parallelism, pushes a trend for clusters of (possibly heterogeneous, scattered) machines - maybe of type SCAN ("Super-Computers At Night") - and for research towards even higher communication cost decrease.

DE PILLIS, L G (Department of Mathematics, Harvey Mudd College, Claremont, USA)

Modeling cancer tumor growth with immune resistance and an optimal control approach to treatment

In a cooperative effort with clinicians and research oncologists, we have been investigating mathematical models of cancer tumor growth. Currently, there are in existence an array of such mathematical models, each of which tends to focus on simulating only one or two important elements of the multifaceted process of tumor growth and treatment. Until now, however, much of observed effects have not been well understood beyond the simplest models. In an effort to better understand how the various aspects of growth and treatment interact with one another, We have created a new mathematical model of tumor growth which incorporates multiple important elements of the growth processes and the effect of their mutual interactions. An additional component of the model is the implementation of optimal control to search for treatment protocols which, in theory, are improvements to the standard protocols in use today. Preliminary results have been well-received, and future directions will be discussed.

DE SIMONE, Valentina (University of Naples & CPS-CNR, Italy)

Parallel computational issues for image processing

In this talk, we survey some of basic ideas about the analysis, design and implementation of algorithms for Image Processing in a parallel environment. We try to explain these concepts by considering the *restoration* of images from degraded observations, whose mathematical model is an integral equation of first kind. Two strategies for introducing parallelism into algorithms will be considered, *the parallelization of the building blocks* and *the domain decomposition*, the first one based on the use of the Fast Wavelet Transform for the numerical solution of the discrete model, and the other based on the use of Total Variation as regularization functional. This is a joint work with L D'Amore, II University of Naples and CPS-CNR, Italy and A Murli, University of Naples and CPS-CNR, Italy.

DEBNATH, Joyati (Winona State University, USA)

Associated pairs via an automated system

It is often desirable to compute the inverse of the multidimensional Laplace transform at a single variable. Such an image function at one variable can be obtained by evaluating the associated transform corresponding to certain types of multidimensional Laplace transform through the Association of Variables. This paper presents new developments of associated transforms through a Mathematical software system (MaSS), which can be used to mechanically generate associated pairs for certain types of functions. The architectural design including the algorithms for the MaSS is discussed. The results of this paper will be useful in mathematical sciences, physical sciences and engineering applications.

DEBNATH, Narayan C (Winona State University, USA)

SGPG: A graph for modelling concurrency

This paper addresses issues related to concurrent programs and develops algorithms for modeling concurrency. The Generalized Program Graph model is extended to define a new graph representation, called Synchronized Generalized Program Graph (SGPG), for representing concurrent programs. Algorithms required to generate SGPG are presented. These algorithms incorporate the concepts of control flow, control and data dependencies, communication activities and synchronization primitives. The inter-module and intra-module data dependencies and control dependencies are described. The proposed algorithms of concurrent programs may serve as a potential tool for the implementation of an automated software system and evaluation of correctness of concurrent programs.

DELGADO-ROMERO, Juan J D (Instituto Tecnológico de Morelia, México)

Robust analysis of physical systems: Application conditions

In this paper we describe some application conditions to guarantee robust stability of physical linear time invariant systems with parametric uncertainty. The parametric uncertainty is given by an interval matrix. We know the stability of a continuous linear time invariant system is given only by A matrix; if the system contains parametric uncertainty, then A matrix can be an interval matrix $A=[L, U]$. The principal motivation of this work is given by the existence of dynamic systems with parametric uncertainty in its models. This is a joint work with Rodolfo González- Garza and Eduardo Hernández-Morales.

DEMEIO, Lucio (Dip. di Matematica "V.Volterra", Università' di Ancona, Italy)

Collisional relaxation of undamped plasma waves

We study numerically the effect of binary collisions on the time evolution of undamped nonlinear plasma waves (BGK modes) by using a newly developed algorithm for the numerical solution of the Vlasov-Poisson system to which we add a collisional term in the Krook form with velocity dependent collision frequency. Our simulations show that these effects as well as the approach towards the statistical equilibrium depend mainly on the local properties of the collision frequency in the vicinity of the phase velocity.

DESERI, Luca (Dipartimento di Ingegneria-Universita' di Ferrara, Italy)

On the response of viscoelastic polymers under finite deformations

A free energy suitable to describe the isothermal behavior of an extensive class of polymeric materials in finite viscoelasticity is presented. Accordingly, a non-linear Boltzmann-Volterra constitutive equation for the Cauchy stress is derived by taking that free energy as potential, whose relaxation function depends on an invariant of a measure of the deformation gradient. For polymers such as polypropilene, poly(methyl methacrylate), epoxy glasses and other materials of industrial interest, undergoing isochoric deformations the constitutive equation derived from that free energy turns out to predict the observed response, even though only few scalar parameters enter in the expression of the free energy. Particular cases of finite deformations are actually investigated. The model is validated in these situations on a variety of homogeneous polymeric materials subjected to simple stress states.

DEVENISH, Benjamin J (University of Newcastle, UK)

A PDF model for dispersed particles with inelastic particle-wall collisions

A simple model is proposed for the phase-space distribution of dispersed, high-inertia particles in a turbulent boundary layer. This model includes a boundary condition describing inelastic particle-wall collisions. Such interactions are characteristic of the riser section of fast (circulating) fluidized beds. A constant coefficient of restitution is assumed and this is shown to lead to a singular distribution of particle velocities at the boundary. A numerical scheme for treating this model is presented and the results compare favourably with those from a random walk simulation for relatively high values of the coefficient of restitution. Asymptotic analysis shows that the one-dimensional steady state distribution exists only when the coefficient of restitution is greater than 0.5. The particle concentration and particle fluctuation energy at the wall, required to formulate boundary conditions for the 'macroscopic' two-fluid models, are calculated as functions of model parameters. The results also illustrate the phenomenon of particle segregation towards the wall in turbulent gas-particulate suspensions, *i.e.* the formation of the near-wall dense layer of particles; the thickness of this layer is also determined as a function of model parameters.

DIAMANTAKIS, Michalis (Centre for Process Systems Engineering, Imperial College, London, UK)

An implicit Runge-Kutta code for large, sparse differential algebraic systems

Large sparse systems of differential-algebraic equations (DAEs) with discontinuities are frequently encountered in application areas. Computer codes for the numerical solution of DAEs are usually based on Backward Differentiation Formulae. However, despite their wide applicability, these codes have some limitations (e.g. they are not very efficient when frequent discontinuities or highly oscillatory modes exist).

Motivated by the efficiency of the L-stable, 5th-order, RadauIIA Runge-Kutta formula we have developed a RadauIIA code for the efficient solution of large, sparse, fully implicit DAEs with discontinuities. In the numerical results and comparisons we present, performed on a wide set of industrial problems, we attempt to demonstrate the efficiency of this new code. This is a joint work with C C Pantelides.

DJURANOVIC-MILICIC, Nada (Faculty of Technology and Metallurgy, Yugoslavia)

A generalized curvilinear path step-size algorithm

In this paper we present a generalization of the second-order step-size algorithm. This generalization is based on so called "forcing functions". It is proved that this generalized algorithm is well defined. A proof of the convergence of the sequence of points generated by the generalized algorithm to a second-order point of the nonlinear programming problem is given.

DOMNYTSKY, Vladymyr (State Kiev University, Ukraine)

On the asymptotic solution of a system of integro-differential equations with lagging argument

An investigation is made of the nature asymptotic solutions in sense Bogolyubov-Mitropolsky for the system of integro-differential equations with lagging argument: 1. Algorithm for the construction of a formal solution in the "resonance" case. 2. Algorithm for the construction a formal solution in th "nonresonance" case. 3. Asymptotic Character of formal solutions. 4. Asymptotic solution in the case of multiple eigenvalue.

DONATINI, Pietro (University of Bologna, Italy)

Natural size distances for comparison of shapes

Natural Size Distances are a new geometrical-topological technique for comparing shapes of manifolds representing objects. They are defined by considering the infimum of a functional Θ over a set of homeomorphisms. Θ measures the maximum change of suitable real functions at corresponding points. The properties of these distances make them interesting for applications in Computer Vision.

DORNINGER, Dietmar (Vienna University of Technology, Austria)

A cellular automaton model for chromosome pairing

In order to simulate the process of homology searching and interlocking of chromosomes in the meiotic cell nucleus we construct a cellular automaton which reflects both the spatial and the temporal behaviour of the chromosomes during meiotic pairing. We investigate the effects of random and biased movements and of different numbers of homology recognition sites on the efficiency of the pairing process and we calculate the probability of interlocking events, i.e. we estimate - also by using analytical methods - how often chromosomes can get trapped between others and hence may cause genetic defects. This is a joint work with G Karigl and J Loidl.

DROZDOVA, Julia (Gubkin State Academy of Oil and Gas, Russia)

Nonlinear interaction of waves in a channel with arbitrary cross-section

The paper deals with linear and nonlinear waves of small amplitude in nonuniform channels. Two classes of channel cross-sections are considered. The first class have narrow domains with sharp variations of the depth while the depth in the channels of the second class varies slowly. The resonant nonlinear interaction of waves is investigated analytically and numerically in the shallow water approximation. The interaction of waves with a solitary wave is studied with the use of the Boussinesq equations. Examples of numerical calculations of waves interaction are given.

DUAN, Jinqiao (Clemson University, USA)

Dynamical systems methods for geophysical/environmental modeling

In this talk, I will present the results on dynamical systems methods for prototypical models in stochastic as well as deterministic geophysical and environmental systems.

DUBINSKY, Andrej Yu (Keldysh Institute of Applied Mathematics, Moscow, Russia)

Mathematical modelling of electron transport and proton transfer in chloroplasts

A mathematical model is constructed of electron transport coupled with proton transmembrane transfer in thylacoids of chloroplasts. It was taken into account that the rate of electron transport is controlled by the value of the intrathylacoid pH hence depends on mechanisms of proton leakage through the thylacoid membrane and on its geometric form. The set of equations which describe the processes of interest contains non-linear and "diffusion" terms. The results are agree with experimental data. This is a joint work with A N Tikhonov. Reference: A.Yu.Dubinskii, A.N.Tikhonov, Regulation of electron and proton transport in chloroplasts... Biophysics, Vol.42, 639, (1997).

DUDZIAK, Marian (Poznan University of Technology, Institute of Combustion Engines and Machine Construction Foundations, Poznan, Poland)

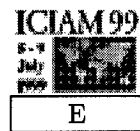
Finite deformations and limit load of elastomer elements

The internal structure of elastomers allows for finite elastic deformations to take place. Breakdown of such non-linear elastic materials or transition into plastic stress state is discussed. The mathematical model and the elastic potential with the material constants determined experimentally are derived and critical conditions based on the Huber-Mises and Tresca material failure theories are specified. As an example, the deformations and critical stresses in some of machine elements loaded in combined way are determined. This is a joint work with Mielniczuk Janusz, Pedagogical University of Zielona Gora, Institute of Technology, Zielona Gora, Poland.

DZIECIELAK, Ryszard (Poznan University of Technology, Poland)

Permeability tensor for heterogeneous porous medium of fibre type

A theoretical model which allows us to determine the permeability of a fibrous porous medium is proposed. Fibres are assumed to be parallel and nonuniform in space and material with a low volume fraction of fibres is considered. The model includes two geometric parameters: the diameter of fibres and the diameter of caverns or fissures inside the bundle of fibres. The tensor of permeability of the porous medium is determined based upon a generalized cell model. The components of permeability tensor depend on two parameters which are determined using experimental data and least-squares approximation. This is joint work with Jan A Kolodziej and Zenon Konczak.



EASTON, Alan K (Swinburne University of Technology, Australia)

Stability of the selective lumped mass scheme for the shallow water equations

The selective lumped mass scheme is an explicit time stepping scheme used by a number of authors for the prediction of tidal flows in coastal seas. As an explicit scheme it has the relatively small computer space requirements but, since it is only conditionally stable, it requires very small time steps. The stability of the scheme has been investigated and new criteria have been developed for the one space dimension case. The relationship of the selective lumped mass parameter and the stability is examined. This is joint work with Sukvinder Goraya and Manmohan Singh.

EGLIT, Margarita E (Moscow State University, Moscow, Russia)

The effect of weak heat-conductivity on propagation of long acoustic waves in mixtures

Mixtures of liquids and gases are considered as inhomogeneous media with typical inhomogeneity scale d . Small amplitude compression waves are studied with typical wave length $L \gg d$. Heat-conductivity in the mixture is taken into account and the homogenization procedure is performed to obtain averaged equations supposing ε and γ tend to zero, where $\varepsilon = d/L$, γ is nondimensional parameter proportional to square root of the typical heat-conductivity coefficient.

The averaged equations are proved to depend essentially on the relations between small parameters ε and γ . In particular, if they are of the same order then the effective equations are integrodifferential.

EGOROVA, Lidia A (Institute of Mechanics, Moscow State University, Moscow, Russia)

Interaction between electron excited nitrogen and non-uniform catalytic surface

The hypersonic dissociated nitrogen flow over a blunt body have investigated. In the specific case of Reaction-Cured Glass surface, experimental data and asymptotic formulas for heating rates were used to develop a model for the gas-surface interaction. The catalytic surface assumed "guided" non-uniform as the adsorbed particles affect one another. It has been considered formation of electronically-excited molecules and atoms on the body surface. Expressions for effective probability of the atomic recombination and for dissociation energy accommodation coefficient have been obtained. The model accounts for a strong dependency of the quantities on pressure, temperature and mixture composition.

EL BADIA, Abdellatif (University of Technology of Compiègne, France)

Some PDE inverse problems from lateral boundary measurements

The first part of this study deals with the identification of a certain coefficient in a multi-dimensional heat equation using a complete set of multiple input sources provided a certain integral average of flux is used as overposed data. The second part deals with a domain identification in an elliptic and a hyperbolic equation from single lateral boundary measurements.

ELISEEV, Kirill Valentinovich (St Petersburg State Technical University, Russia)

Creep analysis at the local nonuniformity of reological properties

Presence of soft layer in some kinds of weldments, which are widely used for the practical applications as the local nonuniformity of reological properties, causes intricate fields of stresses and strains even under uniaxial loading. Using continuum creep damage mechanics, the approach has been developed to carry out analysis of stresses, strains and creep damages fields in connection with the above problem. creep and fracture. It should be particularly emphasized that the finite element user's procedure to simulate creep damage fields was developed.

This is a joint work with Nikolai Shabrov and Yury K Petrenya.

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FABIJONAS, Bruce (National Institute of Standards and Technology, USA)

The computation of special functions in parallel

Many codes exist for the computation of special functions. However, most are old and do not take into account recent advances in computer technology. In particular, few are designed to take advantage of multi-processor or vector machines. We perform a comparative study of computation time by parallel numerical integration of the differential equations associated with the Airy functions, Scorer functions, and modified Bessel functions of pure imaginary order on single, vector, and multi-processor machines. The arguments to these functions are allowed to be complex. This is a joint work with D W Lozier of NIST and J M Rappoport of the Russian Academy of Sciences.

FAGHLOUMI, Chakib (Dpto. de Matemática Aplicada, Univ. Complutense de Madrid, Spain)

Analysis of nonlinear elliptic problem arising in the study of policies on projects alternating the environment

In this paper we study a class of optimization dynamics problems displaying irreversibility that are inspired by questions on the economics of environment management. Much of the discussion concerning biodiversity as well as other aspects of environmental policy focuses on the irreversibility of certain actions that alter the environment. Economists have recently started to study the effect of the ability to delay an irreversible investment expenditure on the decision by firms to invest. In that paper we apply similar reasoning to study the decision to proceed with projects that alter in an irreversible way the environment. The principal lesson is that in analogy to the case of irreversible investments by firms, the decision to start a project when the present value of the expected loss it will cause in the environment equals its expected benefits, is incorrect, even in the absence of risk aversion. This is a joint work with Profesor Jesus Ildefonso Diaz.

FAVELLA, Luigi (Department of Physics, University of Torino, Torino, Italy)

Mathematical model of Eigenfunctions for image Loève-Karhunen reconstruction

It has been proved that the system of eigenfunctions belonging to the Covariance kernel for a very large, symmetry invariant, sample of square tessels from pictorial images, can be considered as a universal system since it allows very good reconstruction of pictorial images with large compression coefficients (L.-K. expansion). The analytical study of the kernel has evidenced that the separable model in two uncorrelated unidimensional Markov processes, is not able to explain the order resulting for from the experimental eigenfunctions from eigenvalues. It is also numerically proved that, in the case of "tessels with circular symmetry" (or better telescopes photographs), the eigenfunctions are Bessel functions, while the eigenvalues are integrals of the spectral function. We have numerical representation of eigenfunctions and show that those obtained from the separable model, may be good approximations of the real ones provided their order is changed by means of perturbative corrections. Finally, we propose general techniques for the analytic solution of homogeneous Fredholm integral equation by means of complex plane integrals in the case of a finite number of spectral singularities; the method may be easily implemented with the help of Mathematica.

FDEZ-GARCÍA, José R (Depto. Matemática Aplicada, Universidade de Santiago de Compostela, Spain)

A finite element contact model for the reduction of Mandibular fractures

We present a frictionless unilateral contact model among three elastic bodies to simulate the reduction of mandible fractures with screwed miniplates based on Michelet's technique. So, the problem derives to a variational inequality which we solve using a tetrahedral finite element discretization and a duality-penalty algorithm. Finally, we show some numerical experiments simulating the stress and displacement fields in some mandibular fractures reduced with one or two miniplates. This is a work joint with J M Viaño and M Burguera, Dpto. Matemática Aplicada. Univ. Santiago de Compostela, Spain.

FEGAN, George R (Santa Clara University, School of Engineering, USA)

A relationship between the compound Poisson distribution and the swap-up distribution

The Swap-Up Distribution which can be applied to both the Secretary Problem and Lamport's Bakery Problem has a probability mass function (p.m.f.) which has been calculated recursively. The distribution may be used to count the frequencies for the Cayley representation of the Symmetric Group $S(n)$. From an examination of a Compound Poisson Problem given by Feller (1950), it is shown that the Swap-Up probability mass function can be derived from the coefficients of a simple polynomial representation for a negative binomial probability mass function.

FELTHAM, Daniel L (UMIST, UK)

Solidification of spheres with application to emulsions

The inward solidification of spheres has important applications in many industrial crystallization processes. Previous theoretical studies have focused upon the inward solidification of pure materials at their freezing temperature. We extend these studies in two important ways: by considering two component solidification (in order to describe materials as diverse as binary organic melts and steel); and by considering the presence of undercooling. Our solutions describe the temperature and composition fields and the evolution of the solid melt interface. We discuss the physical stability of these solutions and present extensions required for the application of our model to crystallization in emulsions.

FENG, Bao-Feng (Kyoto University, Japan)

Numerical computation for stationary travelling-wave solutions of the Kuramoto-Sivashinsky equation: A rational spectral approach

Existing numerical results indicate that the Kuramoto-Sivashinsky (KS) equation, known as a popular prototype for systems which exhibit spatio-temporal chaos, admits three classes (namely, regular shock, oscillatory shock, and solitary wave) of non-periodic travelling-wave solutions and families of multi solutions in each class. However, the details of multi solutions are still unclear because of numerical accuracy. In this work, a rational spectral approach is used to compute these multi travelling-wave solutions. Owing to the high accuracy of the employed method, the new families of regular shock waves are found and the fine-structure of each family is recognized. Furthermore, relations among three classes of solutions are uncovered.

FERNÁNDEZ-GAUCHERAND, Emmanuel (University of Arizona, USA)

Controlled Markov processes with risk-sensitive average optimality criteria

We consider Controlled Markov Processes with (risk-sensitive) long-run average exponential-of-costs optimality criteria. Recently obtained key, and quite revealing, results by the authors are reviewed. Counter-examples to claims in the literature on existence of solutions to the (Poisson) optimality equation are presented, and sufficient conditions for the latter are then given.

FIBICH, Gadi (Tel-Aviv University, Israel)

Dynamic optimal pricing decisions in the presence of reference-price effects

Reference-price is the price a consumer has in mind, to which he compares the shelf-price of a specific product. We formulate a model for optimal pricing strategies in the presence of reference-price effects. The model is based on a new formulation for the 'market reference-price' which is continuous in time. We show that the key parameter of the problem is the Consumer's Life-time Interaction (CLI) parameter, which is roughly the average number of purchases during the planning horizon. Asymmetric effects, oligopolistic competition and boundary-layer formation will also be discussed. This is a joint work with A Gavious and O Lowengart.

FISCHER, Oliver (Bilfinger + Berger Bauaktiengesellschaft, Germany)

Non-linear dynamic behaviour of inclined suspended cables

Starting from a general vector formulation non-linear equations of motion are derived which allow to investigate spatial vibrations of suspended cables including parametric excitation and the interaction with longitudinal resonance effects. Using the principle of virtual displacements, the equations are finally transformed and utilised in a single compact equation of work which in turn can be used effectively as a basis for the solution of non-linear vibration and stability problems of cable structures. As an example of application, the numerical solution is performed for spatial oscillations of inclined cables and the results are compared both with literature and large-scale experiments.

FREDENHAGEN, Sigrid (Institute for Applied Mathematics, University of Hamburg, Germany)

Constrained nonlinear spline-interpolation

A thin stripe of wood (*spline*) which is led through slide bearings will take a form which minimizes the bending energy. In contrast to the problem of bending a beam, here the length of the curve is free. The problem is formulated as an optimal control problem. Further, state constraints as the non-negativity are considered. The necessary conditions of optimal control lead to a system of nonlinear equations. For the non-negativity constraint it can be shown, that no more than one contact point or one boundary arc appears between two interpolation knots. An algorithm for the constrained nonlinear spline and numerical results are presented.

FRIEDLANDER, Ana (State University of Campinas, Brazil)

On the resolution of the generalized nonlinear complementarity problem

Smooth optimization with box constraints is proposed as a strategy to solve the generalized nonlinear problem (GNCP) defined on a polyhedral cone. Theoretical results that relate stationary points of a smooth function to the solutions of GNCP are presented. These results suggest the use of local methods for box constrained minimization for solving GNCP. There is no need to solve difficult subproblems or to calculate complicated projections. Numerical experiments are presented.

FRONTINI, Gloria L (University of Mar del Plata-Intema, Argentina)

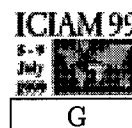
Combining measurements to improve the solution of an inverse problem in polymer latex characterization

The aim of this work is to solve the inverse problem of estimating the particle size distribution of a polymer latex from combining turbidity and scattered light measurements in order to improve the estimations obtained when the measurements were processed independently. The combined problem is a linear inverse problem if absolute measurements were given. However, available measurements are usually relative to an unknown parameter, which should be considered in the mathematical formulation. The non-linear inverse problem that considers this situation is solved in this work. Simulated examples show that the method proposed produces better solutions than those obtained by the application of Phillips' technique in each independent problem.

FURIHATA, Daisuke (Research Institute for Mathematical Science, Kyoto University, Japan)

Finite difference schemes for nonlinear wave equations that inherit energy conservation or momentum conservation property

We propose new general finite difference schemes that inherit the energy conservation or momentum conservation property from nonlinear wave equations, such as the nonlinear Klein-Gordon equation. The most important feature of our procedure is a rigorous discretization of variational derivatives using summation by parts. We show that almost all of energy or momentum conserving schemes that are proposed so far can be treated as particular examples of our scheme. The inherited properties are satisfied exactly and some examples are explicit but symmetric. Because of these properties we can expect that derived schemes are numerically stable and yield solutions with small computation cost and that solutions converge to PDE solutions.



GAIKO, Valery A (Belarussian State University of Informatics and Radioelectronics, Belarus)

Termination principle and its application to Hilbert's 16th problem

Perko's termination principle states that the maximal (global) one-parameter family of multiple limit cycles of a relatively prime, planar, analytic system is either cyclic or terminating either at a singular point, which is typically of the same multiplicity, or on a separatrix cycle, which is also typically of the same multiplicity. We formulate this principle for polynomial dynamical systems considering, in particular, a canonical quadratic system with three field-rotation parameters, prove that the global one-parameter family of multiple limit cycles for such a system cannot be cyclic and apply the principle for solving Hilbert's 16th problem on the maximum number and relative position of limit cycles.

GALIEV, Shamil (University of Auckland, New Zealand)

Resonant amplification of earthquake waves in sedimentary basins and hills

Many cities are built on naturally resonant soil and rock profiles. Resonant amplification of seismic waves in a sedimentary basin lead to the collapse of about 300 buildings in the 1985 Michoacan earthquake. We illustrate nonlinear amplification of seismic waves and demonstrate that localised oscillating earthquake induced waves may be generated on the surface of sedimentary basins and towards at the tops of hills and mountains. (See also Galiev, Sh U et alin Phys. Lett. A 246 (1998) 299). This is a joint work with M J Pender.

GALLICE, Gerard (CEA/CESTA, France)

Positive ROE matrices for Eulerian and Lagrangian MHD equations

It is well-known that the Roe schemes known until now have a major drawback which is to lead to non-admissible solutions. This means that the intermediate states of the associated linearized Riemann problem can have negative densities or pressures. It is shown here that it is possible to construct positive Roe schemes for MHD, both for eulerian and lagrangian coordinates. Furthermore, in lagrangian coordinates, a family of Roe matrices is constructed so that the numerical flux is equal to the continuous flux evaluated at an intermediate state. This family depends on an arbitrary parameter A which represents the sound speed.

GARCIA-PALOMARES, Ubaldo M (Universidad Simon Bolivar, Venezuela)

Parallel conjugate gradient for solving algebraic linear system of equations

Conjugate gradient (CG) methods have become the paradigm for solving linear system of equations. On the other side, projection techniques (PT) for solving a convex feasibility problem are quite robust and can be efficiently implemented in a multiprocessing environment. We report here a nice connection between (CG) and (PT) which leads to a parallel algorithm that split a large system in subsystems of adequate size. One iteration of the algorithm involves approximate solutions of every subsystem by CG techniques. These solutions are reconciled using acceleration schemes that have been highly successful in (PT) (See Ubaldo M. García-Palomares, Francisco J. González Castaño, *Incomplete Projection Algorithms for Solving the Convex Feasibility Problem*, accepted in "Numerical Algorithms"). It is worth to point out that in many cases (CG) does not terminate in the number of finite iterations implied by its well-known theoretical properties. Some remedies are proposed. Preliminary numerical results are reported.

GARCIA-REIMBERT, Catherine (IIMAS-UNAM, Mexico)

Evolution of a hotspot in a cylindrical dielectric material heated by microwaves

We consider the propagation of a temperature front in a cylindrical rod heated inside a semi-infinite waveguide. The energy input is from microwave radiation, and it is assume that can be lost by radiation leakage from the boundary of the rod. The hotspot is treated as a moving boundary layer.

The position of the temperature layer and distributions of temperature and electric field are obtained in closed form and compared with numerical solutions of the full initial boundary value problem giving a very good agreement. This is a joint work with A A Minzoni and N F Smyth.

GASSER, Ingenuin (Institut für Angewandte Mathematik, Universität Hamburg, Germany)

On the vanishing Debye length limit in the drift diffusion model for semiconductors

We discuss the vanishing Debye length limit in the selfconsistent Drift Diffusion model for semiconductors. On the fast initial layer time scale this corresponds to a zero diffusion limit. The limiting problem is a nonlinear hyperbolic system. On the slow timescale the limiting problem reduces to a heat equation. This is a joint work with Peter Markowich.

GAVRILOV, Serge (Institute for Problems in Mechanical Engineering RAS, Russia)

Passage through the critical velocity by a moving load in elastic waveguide: asymptotical solution

The passage through the critical velocity by a load moving along a string on an elastic foundation is considered. We find that pronounced "pit" under the load is beginning to lag behind it after the moment of the overcoming the critical velocity. After this the "pit" moves along the string at the critical velocity and gives rise the pronounced wave front. There are intensive oscillations behind the front. For large values of time we have found the asymptotical solution in the neighbourhood of the front. The stationary phase method has used to obtain the asymptotics.

GAVRILOVA, Elena G (University of Mining & Geology "St. Ivan Rilski", Bulgaria)

Hydroelasticity of thin cylindrical shells with elastic inclusions

A circular cylindrical rigid shell is fulfilled with compressible, irrotational and inviscid fluid. An elastic element (a flexible membrane or an elastic plate) is a part of the cover of the cylindrical shell as the centres of the elastic element and the cover can be coincided or not. Free coupled vibrations of the received hydroelastic system are investigated and the frequency equation is obtained using the Galerkin method. To illustrate the analytical results, some numerical examples are given and discussed.

GAWINECKI, Jerzy August (Institute of Mathematics, Military University of Technology, Warsaw, Poland)

Local existence of the solution to the initial-boundary value problem in nonlinear thermodiffusion in micropolar medium

We proved the theorem about local existence (in time) of the solution to the first initial-boundary value problem for nonlinear hyperbolic-parabolic system of eight coupled partial differential equation of the second order describing the process of thermodiffusion in the three-dimensional micropolar medium. At first, we proved the existence, uniqueness and regularity of the solution of this problem for the linearised system of equation associated with a nonlinear one using the Faedo method, or the method of semi-group theory. Next, we proved (basing on this theorem) an energy estimate for the solution of this problem to the linearised system applying the method of Sobolev spaces. Using the Banach fixed point theorem, we proved that the solution of our nonlinear problem exists and is unique.

GEDDES, John B (University of New Hampshire, USA)

Extracting signals from chaotic laser data

Several experimental groups have demonstrated communication with chaotic lasers. Although the focus has not been on message security, it is believed that the dynamics typically lie on attractors of large dimension which may make it impossible to extract the hidden message using nonlinear forecasting techniques. In this paper, we analyze data from numerical simulations in order to determine what system information is necessary to make unmasking possible. We also comment on results using actual experimental data.

GEORGIEVSKII, Dimitri V (Moscow State University, Russia)

The notion of yield stress for tensor non-linear media

Continuum media where deviator stress tensor and strain rate tensor are connected by tensor non-linear isotropic function, are considered. Material properties of these media essentially depend on both quadratic invariant (maximal strain rate or intensity) and cubic invariant of strain rate tensor. The classical notion of yield stress that is well-known in viscoplasticity of quasilinear solids, is generalized for tensor non-linear media. The algorithm of this yield stress obtaining in case of polynomial material functions is derived. Particular attention is given to potential dependence of stresses and strain rates.

GERVASIO, Paola (Department of Electronics for Automation, University of Brescia, Italy)

Homogeneous and heterogeneous coupling for 2D viscous incompressible flows via domain decomposition methods

Some new domain decomposition methods are proposed and analysed for coupling different kind of equations for the simulation of incompressible flows. One motivation is to develop parallel algorithms, the other is to provide an efficient way to handle "far field" boundary conditions through flow models of reduced complexity. In particular, the following models are considered: - The Oseen equations (homogeneous domain decomposition approach); - The coupling between Navier-Stokes equations and Oseen equations (heterogeneous domain decomposition approach). In both cases the mathematically admissible transmission conditions at subdomain interfaces are determined, then suitable iterative procedures among subdomains are proposed. They involve the successive resolution of local subproblems at subdomain level. A convergence analysis of these domain decomposition techniques for finite element approximations is carried out. Some examples of applications of the method are presented for both finite element and spectral element approximations. This is a joint work with Alfio Quarteroni and L. Fatone.

GIOVINE, Pasquale (Dipartimento di Meccanica dei Fluidi ed Ingegneria Offshore, Università di Reggio Calabria, Italy)

Diatomic continua: balance equations and constitutive relations

The balance equations for a binary mixture are specified as is appropriate to cover the case of diatomic crystalline systems. Use is made of an approximation method similar to one proposed by Signorini within the theory of elasticity by supposing that the relative motion between the phases is infinitesimal. Comparisons are also stated with existing theories for the dynamics of diatomic media.

Moreover, the constitutive equations for a mixture of elastic bodies in absence of diffusion are adapted to the partially linearized case here considered and the representation theorems for the constitutive fields are applied to obtain the final expression of dynamical equations in the form which appears in theories of continua with vectorial microstructure.

GOFFIN, Jean-Louis (McGill University, Montreal, Canada)

Multiple cuts in the analytic center cutting plane method

We analyze the p -cuts generation scheme in the analytic center cutting plane method which uses the optimal primal and dual updating direction. The new primal and dual directions use the variance-covariance matrix of the normals to the new cuts in the metric given by Dikin's ellipsoid. We prove that the recovery of a new analytic center from the optimal restoration direction can be done in $O(p \log(p + 1))$ damped Newton steps, where p is the number of new cuts added by the oracle. This is joint work with JP Vial.

GOLUBITSKY, Marty (University of Houston, USA)

Animal gaits and coupled oscillators

Collins and Stewart pointed out that the characteristic gaits of quadrupeds — walk, trot, pace, bound, etc. — can be described by spatio-temporal symmetries of periodic functions. For example, when a horse paces it moves both left legs in unison and then both right legs and so on. This form of motion is determined by two symmetries: (1) Interchange front and back legs, and (2) swap left and right legs with a half-period phase shift. Biologists postulate the existence of a central pattern generator (CPG) in the neural system which sends periodic signals to the legs. These CPGs can be thought of as electrical circuits that produce periodic signals and can be modelled by coupled systems of differential equations with symmetries based on permutation of the legs. In this lecture we discuss animal gaits and describe how periodic solutions with prescribed spatio-temporal symmetry can be formed by Hopf bifurcation in systems with symmetry. We then show how to construct coupled ODE systems that will naturally produce periodic solutions with the symmetries of quadrupedal gaits. This research is joint with Luciano Buono, Ian Stewart, and Jim Collins.

GOURLAY, Tim P (University of Adelaide, Australia)

The Maximum Sinkage of a Ship

A ship travelling in shallow water is usually subject to downward forces which cause it to sink lower in the water, increasing the risk of grounding. The amount of sinkage increases with the ship's speed until it reaches a maximum at just below the shallow-water wave speed. For ships capable of travelling at these speeds, the maximum sinkage can be dangerously large. Recent work done in conjunction with Prof. E. O. Tuck has resulted in accurate methods for predicting the maximum sinkage. These use dispersive slender-body methods, both for general depth and in the shallow-water limit.

GRAHS, Thorsten (Institut für Angewandte Mathematik, Universität Hamburg, Germany)

Nonlinear anisotropic artificial dissipation for numerical approximations of conservation laws

We employ a nonlinear anisotropic diffusion operator like the one used as a means of filtering and edge enhancement in image processing, in numerical methods for conservation laws. It can be shown that algorithms currently used in image processing are very well suited for the design of nonlinear high-order dissipative terms. In particular, we stabilize the well-known Lax-Wendroff formula by means of a nonlinear diffusion term. This is a joint work with Andreas Meister and Thomas Sonar.

GRANDGIRARD, Virginie (Association Euratom-CEA, France)

Free boundary Tokamak plasma equilibrium computation in an infinite domain

In high temperature tokamak plasmas, the pressure gradient forces are balanced by the interaction of magnetic fields with the currents flowing in the plasma. Coupled finite element/boundary integrals methods are used to compute the equilibrium of a plasma in an infinite domain. Direct (Woodbury+Cholesky) and iterative (preconditioned BCG and GMRES) methods are tested to solve the non-symmetric system which arises from the free boundary nature of the problem. These methods are implemented in the Cedres object-oriented code written in C⁺⁺. The results of comparison between direct, sequential and parallelised iterative methods will be presented.

GRANDITS, Peter (Statistical Laboratory, University Cambridge, UK)

Leland's approach to option pricing: the evolution of a discontinuity

In 1985, Leland introduced a theory for hedging and pricing a call option with transaction costs. Recently (1997) Kabanov and Safarian were able to give an explicit (up to a double integral) expression of the limiting (the length of revision intervals tending to zero) hedging error, if one uses Leland's hedging strategy.

It depends on the path of the stock price only via its value at expiry S_T . We prove that the limiting hedging error, considered as a function of S_T , exhibits a removable discontinuity at the exercise price. Furthermore, we provide a quantitative result describing the evolution of the discontinuity, which shows that its precursors can be observed also in cases of reasonable length of revision intervals. This is joint work with W Schachinger.

GRANDOTTO, Marc (DRN/DEC/SECA CEA Cadarache, France)

Two phase flows numerical analysis with liquid and gas momentum equations

This work takes place in steam generators flows studies and we consider herein steady state 3D flows. The main goal is to improve the modeling of kinetic imbalance between the phases. We present a method that solves the mixture (liquid-gas) mass and enthalpy equations, and two momentum equations: the one for the mixture and the one for the gas. This choice is equivalent of solving the gas and the liquid momentum equations, but it is better suited to the Chorin projection method used for the pressure calculation. (cf. M. Grandotto, P. Obry, European Journal of Finite Elements, vol.5, 1/1996 and P.M.Gresho, S.J.Chan, Int. J. Num. Methods in Fluids, 11, 1990). Solving two momentum equations instead of solving the only one for the mixture introduce the use of correlations for the gas-liquid friction, avoid the use of a correlation for the drift velocity and open the way to a finer analysis of the relative dynamic behavior of each phase.

GRIKUROV, Valery (St Petersburg University, Russia)

High-frequency asymptotics in the direction of total-reflection angle over convex interface

The problem is to obtain high-frequency asymptotic formula for electromagnetic field which is reflected from convex (in effective sense) interface in directions close to total-reflection angle. The difficulty here is an interference between reflection wave and head wave near its origin.

We suggest an effective formula for inhomogeneous media, arbitrary interface and both monochromatic and modulated waves. The essential part of this formula is the new special function (in form of contour integral) which doesn't depend on details of the problem. For limit cases of plane interface and/or large distances from the interference head wave' origin our formula is reduced to previously known ones.

GROSS, Laura K (The University of Akron, USA)

Stability of uniform bend Fréedericksz configuration in nematic liquid crystals

One of the interesting phenomena in the physics of liquid crystals is the formation of stable structural patterns in confined nematics. Competition between elastic inner forces and either external fields or surface anchoring forces produce these patterns. The most prominent example of a field-induced molecular structure is a uniform Fréedericksz configuration in a thin nematic film. We discuss the stability of this configuration in highly anisotropic materials. We show that the Fréedericksz transition in a bend geometry is at least two-dimensional, and it occurs at field strengths lower than the known classical threshold. We also discuss the corresponding bifurcation diagram.

This is a joint work with D Golovaty, S I Hariharan and E C Gartland, Jr.

GRØVER, Bent (Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK)

Acoustic waves in locally stratified media

We present a new effective medium theory for acoustic waves in heterogeneous media, where the material properties vary substantially on a fine length scale vertically. In contrast they exhibit a slow variation in the lateral directions. Exploiting the smallness of the ratio between the vertical and the lateral length scales, we apply a multiple scales technique together with an average, with respect to the fine scale variable, to deduce a set of averaged equations. The first order term gives us the effective medium solution. Beyond the effective medium theory, the implications of the second order correction are illustrated numerically.

GRUND, Friedrich (Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany)

Pivot strategies for direct linear solvers

Direct methods for the numerical solution of linear systems with unsymmetric sparse matrices are considered. Different strategies including a new one are studied. For solving several linear systems with the same pattern structure a pseudo code is generated. The pseudo code can be advantageously adapted to parallel computers. Using the pseudo codes results in a fast second factorization. Numerical results are given for the linear solvers GSPAR and SuperLU with different pivoting strategies. The solver GSPAR with the new pivoting strategy shows a fast first factorization. GSPAR is successfully applied to the dynamic process simulation of complex chemical production plants.

GRUNDY, Robert E (School of Mathematical Sciences, University of St Andrews, UK)

Blow-up solutions of the Navier Stokes equations

We consider solutions of the Navier Stokes equations in 2 and 3 dimensions which blow-up in finite time. Using a combination of numerical and asymptotic analysis we give the blow-up rate together with the solution profile close to the blow-up time. Various features of the numerical solution are shown to compare well with the asymptotic structure. This is a joint work with R McLaughlin.

GUHL, Florent (Cemagref, France)

Continuity constraint in optimization of water supply

The optimization of production and transport costs in a drinking water network has been modeled using various operational research methods in recent years. In certain networks, there exists a constraint, which has not yet been incorporated into this type of model. The constraint is associated with the operating conditions of the water treatment plant. To avoid problems with water quality, a water works must be able to operate continuously. This problem is difficult to solve because one cannot apply the Bellman's principle of optimality.

To take account of this extra operating constraint, we propose a method based on linear programming with mixed variables. This method provides satisfaction by maintaining computing times compatible with real time network management.

GUO, Ben Yu (Shanghai University, China)

Jacobi spectral approximations to singular differential equations

Jacobi approximations in certain Hilbert spaces are investigated. Several weighted inverse inequalities and Poincaré inequalities are obtained. Some approximation results are given. Singular differential equations are approximated by using Jacobi polynomials. This method keeps the spectral accuracy.

GVOZDOVSKAYA, Natalia (Institute for Problems in Mechanics, Russian Academy of Sciences, Russia)

The structure of quasitransverse waves in a composite - elastic media with internal structure

The structure of quasitransverse shock waves of small amplitude in anisotropic elastic medium with internal structure, that causes wave dispersion, is investigated. The presence of dispersion is modeled by introduction of terms with high order derivatives into the equations of elasticity, and dissipation is presented by viscous terms. The requirement of continuous structure existence leads to intricate construction of the set of admissible discontinuities. Substantial part of the shock adiabat consists of the set of short intervals and isolated points, their number increasing with decrease of viscosity. This is a joint work with Prof Andrey G Kulikovskii, Steklov Mathematical Institute, Russian Academy of Sciences.

GYURKOVICS, Eva (Budapest University of Technology, Hungary)

Nonlinear receding horizon control for discrete-time uncertain systems

This paper presents a receding horizon control scheme (also referred to as model predictive control or moving horizon control) for nonlinear discrete-time systems with control constraints that guarantees asymptotic closed-loop stability. A necessary and sufficient condition is given for the objective functional to be minimized that ensure the monotonicity of the corresponding value function. The method is a generalization of the methods of Allgower, Chen (1998), De Nicolao et.al.(1997). The receding horizon control is supplemented with an additional control term obtained by a nonquadratic Lyapunov function of the nominal system to improve its robustness. The results are illustrated by examples.

HA-DUONG, Tuong (Universite de Technologie de Compiegne, France)

On the inverse source problem from boundary measurements

We consider the problem of determining a source term from boundary measurements in an elliptic problem. In general, this source is unattainable except for its harmonic component. We then turn ourselves to the problem in some special cases when *a priori* information is available : (1) when separation of variables is possible and one factor of the product is known ; (2) in the case of a domain source of cylindrical geometry, when the area of the base is known.

Our method is based on the *reciprocity gap functional* already used by other authors in the problem of identification of a crack. This is a joint work with Abdellatif El Badia, University of Technology of Compiegne, Division of applied Mathematics, France.

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HABERMAN, Richard (Southern Methodist University, USA)

Slow passage through a saddle-center bifurcation

Slowly varying potentials are analyzed. Away from homoclinic orbits, strongly nonlinear oscillations are obtained using averaging. Usually solutions pass through a double homoclinic orbit before the saddle-center bifurcation. For slow passage through the homoclinic orbit associated with saddle-center bifurcation, solutions consist of a large sequence of nearly saddle-center homoclinic orbits connecting autonomous nonlinear saddle approaches, and the change in action is computed. However, if one saddle approach has particularly small energy, then it instead satisfies the nonautonomous first Painleve transcendent, and the solution may also make a transition to small oscillations around the center.

HACIA, Lechoslaw (Institute of Mathematics, Poznan Technology University, Poznan, Poland)

On iterative-collocation methods of solving Volterra-Fredholm integral equations

Volterra-Fredholm integral equations by iterative method with corrections based on interpolation polynomials with chosen collocation points are solved. Presented corrections can be determined as interpolation polynomials of two variables or as interpolation polynomials of spatial variable of the Lagrange's type. Considered equations so-called mixed integral equations play very important role in the theory of parabolic initial-boundary value problems and various biological and technological problems. The convergence of studied algorithms is proved and an error estimate is established. Presented methods by numerical examples are illustrated.

HACKBUSCH, Wolfgang (University of Kiel, Germany)

Fast arithmetic with hierarchical matrices

A class of matrices (hierarchical matrices) is introduced which have the following properties. (i) They are sparse in the sense that only few data are needed for their representation (data-sparsity). (ii) The matrix-vector multiplication is of almost linear complexity. (iii) In general, sums and products of these matrices are no longer in the same set, but their truncations to the hierarchical matrix format are again of almost linear complexity. (iv) The same statement holds for the inverse of an hierarchical matrix.

The construction of hierarchical matrices is explained for the application to discrete integral operators in one to three spatial dimensions.

HAMEL, François (CNRS, University of Paris VI, France)

Conical-shaped solutions of semilinear elliptic equations in \mathbb{R}^N

We have studied the solutions (c, u) of the equation $\Delta u - c\partial_{x_N}u + f(u) = 0$ in \mathbb{R}^N , which arises in models for Bunsen burner flames. The level sets of the unknown functions u are conical-shaped with a fixed aperture α with respect to the direction $(0, \dots, 0, -1)$. We have emphasized this problem under several definitions for the asymptotic "conical" conditions. By using the sliding method, we have especially proved a non-existence result if $\alpha > \pi/2$, and several existence and monotonicity results and a meaningful formula relating the speed c and the angle α if $\alpha \leq \pi/2$. This is a joint work with A Bonnet and R Monneau.

HANSEN, Olaf (Fachbereich Mathematik, Johannes Gutenberg-Universität Mainz, Germany)

Solving numerically the heat equation in unbounded domains in \mathbb{R}^2

We use the method of Rothe and a single layer potential for the numerical solution of the heat equation outside of a bounded domain Ω in \mathbb{R}^2 . This method was proposed by R Chapko and R Kress.

We assume that the domain Ω has a polygonal boundary. To deal with the singularities of the solution of our first kind integral equation we use a special parametrization for the boundary. Numerical results are presented.

HARPER, John F (Victoria University of Wellington, New Zealand)

Why bubbles rise anomalously slowly in water with air present

In water in contact with air, atmospheric carbon dioxide dissolves to give a very dilute solution of H^+ and HCO_3^- ions; the resulting double layer is of order 300 nm thick. With a potential difference across the layer of about 0.26 V, the contribution to surface pressure is very small. However, the author suggested in 1974 that the flow near the rear stagnation point of a rising bubble might increase the surface pressure locally, and detectably reduce the speed of rise. That suggestion is now confirmed theoretically; it explains a long-known oddity of bubbles rising in water.

HARRIOTT, George M (Air Products and Chemicals, Inc)

Finite element heat exchanger computations

Multi-stream heat exchanger models are comprised of energy balances in which energy is carried along streams by convective terms and distributed among streams by algebraic terms. The rapid redistribution of energy in highly efficient exchangers leads to large "pinched" regions over which temperatures are nearly constant. In this limit, computational design requires resolution of small thermal differences between streams within pinched regions as well as boundary layers at the ends. A SUPG finite element implementation is presented here that eliminates wiggles in the pinched region characteristic of symmetric discretizations and facilitates convergence. Consistent representation of convection, afforded by SUPG, is shown to be essential even though the solution is dominated by algebraic terms in the model. An example will be also given of heat exchange to food freezing processes in which conduction across the streamlines is significant and anisotropic weights are required.

HASEGAWA, Hidehiko (University of Library and Information Science, Japan)

Preconditioner's effects versus quadruple precision operations for Krylov subspace methods

Some preconditioners are required in applying Krylov subspace methods to solve substantially large linear systems. However, it is very difficult to implement good preconditioners efficiently in distributed parallel computing environments. The authors propose to incorporate quadruple precision arithmetic operations for such powerful environments instead of preconditioning. It is simple to implement, and allows smooth convergence. The authors show in which cases and how pure Krylov subspace methods in quadruple precision are more effective than preconditioned Krylov subspace methods in double precision. This is a joint work with K Abe and S L Zhang.

HATAUE, Itaru (Department of Computer Science, Kumamoto University, Japan)

Analyses of structure of spurious solutions in direct simulation of flow problem

In the present study, we analyze the nonlinear qualitative structure of asymptotic numerical solutions calculated by solving the Navier-Stokes equations directly. Some kinds of finite difference schemes are applied to the incompressible Navier-Stokes equations. Explicit method and the well-known marker-and-cell(MAC) method are used. The model adopted in the present study is the flow around two-dimensional circular cylinder. The dependence of the temporal discretization parameter, Δt , and the dependence of schemes on structure of asymptotic numerical solutions are discussed in several Reynolds numbers. Both of flow visualization results and nonlinear dynamics approaches are utilized in order to analyze the structure in detail. For the nonlinear dynamics approaches, time series of the drag coefficients are used. The attractors are reconstructed from those time series and their nonlinear characteristics such as the correlation dimension and so on are analyzed.

HEBERMEHL, Georg (Weierstrass Institute for Applied Analysis and Stochastics, Germany)

Simulation of microwave integrated circuits and multi-chip modules

The scattering matrix describes the properties of the circuits on transmission lines in terms of their wave modes and is computed from the electromagnetic field using a three-dimensional boundary value problem of Maxwellian equations in the frequency domain. Absorbing boundary conditions can be used for open problems. Using a finite-volume method the boundary value problem can be solved by means of a two-step procedure. An eigenvalue problem for non-symmetric complex matrices yields the wave modes. The electromagnetic fields are achieved by the solution of large-scale systems of linear equations with indefinite symmetric complex matrices.

This is a joint work with Rainer Schlundt, Horst Zscheile, Wolfgang Heinrich.

HEDRIH, Katica (Faculty of Mechanical Engineering University of Nis, Yugoslavia)

Vectors connected to a point and to an oriented axis or to an oriented plane with applications

The vectors connected to a point and to an oriented axis or to an oriented plane are considered as their tensor properties. By using these vectors the body mass moment vectors for the point and oriented axis, as well as a vector of the total strain for the point and for the oriented deformable body line element are defined. By using these vectors, the body mass moments state, as well as the deformed body strain state are considered in the analogy with the analogous model of the stressed body stress state. By using these vectors the model of the stationary state of the body random vibration is defined. Spectral density vector of vibrational state in the current point for the oriented direction as well as the corresponding correlation vector are introduced. By using these introduced vectors: for the body mass moment state, for the strained deformable body strain state, for the stressed deformable body stress state, and for the body random vibration stationary state, the analogy between these states is considered. The kinetic parameters analysis of the gyro-rotor dynamics is made.

HEGLAND, Markus (Australian National University, Australia)

Scalable thin plate splines

Recent data analysis problems (e.g. data mining), are characterised by millions of data points and high dimensionality. Radial basis functions provide good approximations but lead to dense linear systems. The computational challenge is due to the fact that the number of unknowns equals the number of data points.

In this project the radial basis function approximations are approximated themselves with finite elements on very fine grids. The approach has a complexity comparable to finite element surface fitting and is scalable in the number of data points. This is joint work with Irfan Altas, Kevin Burrage, Steve Roberts and Roger Sidje.

HEIL, Matthias (Department of Mathematics, University of Manchester, UK)

Airway closure - liquid bridges in strongly buckled elastic tubes

Fluid-elastic instabilities of the liquid film which lines the airways of the lung can lead to the formation of occluding liquid bridges. We study the quasi-steady deformation characteristics of such occluded airways. Non-linear shell theory is used to describe the large deformations of the airway in response to a slowly varying external (=pleural) pressure and to the loads due to the surface tension of the liquid bridge. The governing equations are solved by Finite Element methods.

Parameter studies predict the occluded airway to collapse into a strongly buckled equilibrium configuration in which large parts of the opposite walls are in contact. The deformation characteristics show a pronounced hysteresis in the collapse/reopening cycle. The implications for the airway collapse/reopening problem will be discussed.

HEITZER, Michael (Institute of Safety Research and Reactor Technology, Forschungszentrum Jülich GmbH, Germany)

Large scale nonlinear optimization for FEM-based limit and shakedown analysis

Limit and shakedown theorems are exact theories of classical plasticity for the direct computation of safety factors or of the load carrying capacity of engineering structures under constant and varying loads. The realistic discretisation with Finite Element Methods (FEM) leads to large scale optimization problems. General mathematical optimization methods cannot solve these problems in sufficient time. A basis-reduction technique is used to obtain smaller problems which can be solved effectively by sequential quadratic programming methods. The approach needs considerably less input data and computer time than incremental plastic analyses and is applied to complex structures.

HERRERO, Henar (Universidad de Castilla-la Mancha, Ciudad Real, Spain)

Theoretical study of the bifurcations of a Bénard-Marangoni problem

We prove the existence of a stationary bifurcation in a Bénard-Marangoni problem in a finite 3D box with infinite Prandtl number. The bifurcations have been studied only partially theoretically in this case due to the difficulty of the boundary conditions that has been overcome taking operators with integrals on the boundaries. Also the kernel of the linearization is not necessarily one-dimensional and we have generalized the Crandall-Rabinowitz's theorem to cover this situation. This is a joint work with R. Pardo.

HETTLICH, Frank (Institut für Angewandte Mathematik, Universität Erlangen-Nürnberg, Germany)
On an inverse obstacle problem for the heat equation

The inverse boundary value problem of recovering the shape of an obstacle contained in a bounded domain in two spatial dimensions and separating two distinct heat sources is considered. The knowledge of the initial temperature and the temperature on the exterior boundary in a time interval is assumed. The overdetermined data of measuring the heat flux at certain points on the exterior boundary is used to reconstruct the shape of the obstacle. A uniqueness result and an iterative algorithm solving this severely ill-posed nonlinear problem are presented.

HIRANO, Hiroyuki (Okayama University of Science, Japan)

The two-step preconditioned iterative method

In this talk, we propose a two-step preconditioning matrices $(I+S(\alpha))$ and $(I+BU)$. And we discuss the convergence property of this method for H-matrices. Usually, the matrix-matrix multiplication requires a number $O(n^3)$ of arithmetic operations. So, we propose an algorithm to decrease the arithmetic operations from $O(n^3)$ to $O(n^2)$. Numerical examples are also given, which show the effectiveness of our algorithm.

HIRAYAMA, Hiroshi (Kanagawa Institute of Technology, Japan)

A variable and multiple-precision arithmetic package for C++ language

A variable and multiple-precision arithmetic system consist of integer, rational floating point and complex number has been developed using standard C++ language. These numbers are represented as classes in C++ language. Therefore it is very easy to write a program for a multiple-precision and to convert C or C++ source code to multiple-precision one because these numbers can be treated as intrinsic numbers. We also developed some numerical software with arbitrary precision such as numerical quadrature, linear equation, algebraic equation, etc.

HOÀNG, Việt Hà (Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK)

Singularly perturbed Dirichlet problems in domains perforated randomly by holes of different sizes

We study the problem $-\varepsilon\Delta u^\varepsilon + u^\varepsilon = f$ in a domain Ω_ε in \mathbf{R}^N , which is obtained by perforating randomly from a bounded domain Ω approximately $m_i\varepsilon^{-q_i}$ holes whose size is of order ε_i^2 ($N=3$) and $\exp(-a\varepsilon^{-p_i})$ ($N=2$), according to a positive probability density function $V_i(x) \in C^1(\bar{\Omega})$ ($i=1, \dots, n$). The $L^2(\Omega)$ limit of u^ε in probability in the space of holes' configurations when $\varepsilon \rightarrow 0$, which depends on p_i and q_i and an order of convergence are presented. Results of Le Gall on fluctuation of the Wiener sausage and Sznitman's long time asymptotics of the shrinking Wiener sausage together with the Feynman-Kac formula are employed.

HOCKING, Graeme C (Murdoch University, Perth, Australia)

Modelling an ultrasonic nebulizer

A nebulizer is a device which atomises medicines for inhalation directly into the lungs. The 1998 Australian Maths-in-Industry study group studied the problem of improving the performance of a medicinal nebulizer which is driven by an ultrasonic jet which flows upward through a central chamber. This device is much smaller than conventional air-jet and other ultrasonic nebulizers, and has great potential to improve the quality of drug delivery. The device and its advantages and disadvantages will be described. The suggestions of the MISG will be presented along with some subsequent research. There are a number of interesting aspects to this problem which cover a range of different areas of fluid mechanics.

HOFMANN, Bernd (Faculty of Mathematics, Technical University of Chemnitz, Germany)

Stability rates for ill-posed problems with compact and noncompact operators

The purpose of this paper joint with G.Fleischer (Chemnitz) is to formulate quantitative measures for the strength of ill-posedness of linear inverse problems $Ax = y$ in Hilbert spaces with compact and noncompact operators A , where the range $R(A)$ of A is not closed. From our considerations it seems to follow that the problems with noncompact operators A are not in general less ill-posed than the problems with compact operators. We motivate this statement by comparing the approximation and stability behaviour of discrete least-squares solutions and the growth rates of Galerkin matrices. In detail, we compare compact convolution operators and noncompact multiplication operators with respect to stability rates and convergence properties of the Tikhonov regularization method.

HOGAN, S John (University of Bristol, UK)

Local analysis of C-bifurcations in n-dimensional piecewise-smooth dynamical systems

C-bifurcations (also known as border-collision bifurcations) can occur when the trajectory of a dynamical system leaves one section of phase space and enters another. Different dynamics occur either side of the border between the two areas. Such systems are widespread in engineering (such a aeroelastic structures with freeplay). An analytical framework to describe these bifurcations appeared in the Russian literature over twenty years ago. This paper brings together these results in a more complete form. First a typical C-bifurcation scenario is presented. Then an appropriate local map is derived & used to obtain a set of conditions to describe all possible co-dimension 1 bifurcations. A sudden jump to a chaotic attractor is shown. The method is then applied to a two-dimensional map & to a set of first-order ODEs.

This is joint work with M di Bernardo, M I Feigin, Volga State Academy of Water Transport, Nizhny Novgorod, Russia and M E Homer, University of Bristol.

HOODA, D S (Department of Mathematics & Statistics, CCS Haryana Agricultural University, Hisar, India)

Generalized measures of useful directed-divergence and information improvement with applications

A new generalised measure of useful directed-divergence based on $m-1$ probability distributions and a probability distribution closest to these probability distributions has been proposed and studied. These techniques have been applied to some problems of crop production, export and industry. A generalised measure of useful information improvement has been developed and applications include pattern recognition and assesment of balanced military requirements for a country.

HORNE, Rudy L (University of Colorado USA)

A comparison between lumped and distributed filter models in WDM soliton systems

In this talk, the effects of a lumped vs. a distributed approach to filtering in models for wavelength-division multiplexing (WDM) solitons systems is examined. We use this comparison to obtain some results about collision induced timing jitter in relation to soliton pulses in an optical fiber.

HSU, Jyh-Ping (Department of Chemical Engineering, National Taiwan University, China)

Stability of a colloidal dispersion: charge regulation/adsorption model

The stability of a colloidal dispersion is one of its basic properties which is of fundamental significance in areas such as wastewater treatment and semi-conductor processing. To estimate its value, the electrical interactions between two charged particles need to be calculated. Here, we consider the case of two spherical particles the surface of which contains dissociable functional groups and/or is capable of exchanging ions with surrounding liquid phase. The linearized Poisson equation describing the spatial variation of electrical potential is solved, and the solution obtained used to estimate the electrical interaction energy between two particles.

HUZAK, Miljenko (Department of Mathematics, University of Zagreb, Croatia)

A generalization of some diffusion growth models

A stochastic diffusion growth model is introduced by stochastic differential equation (SDE) in a way that generalizes Gompertz, logistic and Bertalanffy growth models. It follows that there exists continuous, pathwise unique and stable solution of the given SDE. Some properties of trajectories of the growth process are derived. Especially, the problems of maximum likelihood estimation of the unknown drift parameters and model selection based on continuous observations are discussed.

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IKUNO, Soichiro (University of Tsukuba, Ibaraki, Japan)

Numerical method for MHD equilibrium of Trooidal plasma in arbitrary shaped FC

The numerical method for MHD equilibrium configuration of low-aspect-ratio toroidal plasma in the arbitrary shaped flux conserver (FC) is investigated. The equilibrium configurations of toroidal plasma with the bias coil is determined by use of combination of FDM and BEM. In general, shape of the FC is complex. Therefore, the boundary-fitted curvilinear coordinate system is constructed and FDM is used by its means in the method. Since the combination method is performed FDM and BEM alternately, it takes long time to determine the equilibrium configuration. In the present study, improvement of the method is also investigated.

This is a joint work with Makoto Natori and Atsushi Kamitani.

IL'ICHEV, Vitaly G (Rostov State University, Russia)

Ecology-evolutionary models: theory and application

The development the new models of water ecological systems, which allow consider the dynamic of population sizes and adaptation of biological parameters simultaneously. This methods include the relatively small number of variables in comparing to the traditional ecology-evolutionary models. The developed models were used to solve the following actual problems: i) investigations the climate effects on the water ecosystems taking into account population microevolution; ii) analysing the adaptations of river's ecosystem to lake's one. Reference. Il'ichev V.G. 1996. Mathematical problems of biological competition theory in changing environment//Ecological modelling.93.191-201.

ILIESCU, Traian (University of Pittsburgh, USA)

Numerical analysis for large eddy simulation

This paper presents new continuum models arising in the study of Large Eddy Simulation for turbulent flow. In particular we present a new closure approximation which better attenuates small scales. Numerical analysis for the discretization of these new models is also provided, including a posteriori error analysis in the large eddies.

IRAGO, Hipólito (Dpto. Matemática Aplicada, Universidade de Santiago de Compostela, Spain)

Convergence of high frequency modes in thin rods

This work is concerned with the asymptotic analysis of the high frequency modes in three-dimensional linear elasticity of thin rods as diameter of the cross section tends to zero. Using a combination of asymptotic technics of Kerdid[1995] and Trabuco-Viaño[1996] for the low frequencies (bending) we prove the existence of increasing families of three-dimensional eigenvalues converging to eigenvalues of classical one-dimensional stretching and torsion vibration models. This is a joint work with N Kerdid, Université P. et M. Curie, Paris, France, and J M Viaño, Universidade de Santiago de Compostela, Spain.

ISMAIL, Mohammad S (King Abdul Aziz University, Saudi Arabia)

A predictor-corrector scheme for the sine-Gordon equation

A predictor-corrector scheme is developed for the numerical solution of the sine-Gordon equation. Using the Method of Lines (MOL) approach the sine-Gordon equation is transformed into an approximating non-linear system of Ordinary Differential Equations. Numerical results are presented which demonstrate the efficiency and accuracy of the method. This is a joint work with Abdul Q Khaliq, Western Illinois University, USA

ITOH, Shoji (University of Tsukuba, Ibaraki, Japan)

Some fast methods for periodic block pentadiagonal linear systems on vector processor

Applying the fourth order accuracy's AF method to compressive CFD, one must simultaneously solve a lot of linear systems. In the case of Dirichlet boundary conditions, the coefficient matrices are block pentadiagonal. Here, a new effective method "Rotated Alternative LU decomposition" is proposed. In the case of periodic boundary conditions, this method can not be applied directly. However, Sherman-Morrison-Woodbury formula can be used as a preconditioner of Rotated Alternative LU decomposition to solving these periodic boundary systems. Several numerical experiments show that these methods are faster than the original LU decomposition. This is a joint work with S L Zhang, M Natori and H Hasegawa.

ITOH, Toshiaki (The University of Tokushima, Japan)

Discretization of ordinary differential equations that have exact solutions

We classified the exact discretization procedures for *ordinary differential equations* (ODTEs) which have exact solutions or what we call integrable by quadrature. For this article, we referred to nearly 5000 ODTEs that are included in recent published handbook of exact solutions for ODTEs. It was also treated why we can get *ordinary difference equations* (ODCEs) that have same solutions to correspond ODTEs in most of the cases. Moreover we refer to relation between singularity confinement conditions and eliminating processes of integral constants. We also considered probability of representation for special functions by OTCEs. In this article, multi-boundary problems, singular properties and singular points relate to integrability of OTCEs are also treated.

IVANOV, Anatoli F (Department of Mathematics, Pennsylvania State University, USA)

Stable solutions of differential delay models

Mathematical modeling of a large variety of real life phenomena results in differential delay equations. Stable solutions play an important role as they are usually the ones representing actual dynamics. We address two aspects of the stability in differential delay equations: global stability of equilibria and asymptotic stability of periodic solutions. A number of differential delay models are shown to be globally stable if they can be put into an appropriate form of singular perturbations of discrete globally attracting maps. Asymptotically stable periodic solutions are shown to exist in differential delay models with a number of symmetries, the so-called symmetric differential delay equations. The problem of the stability of periodic solutions in even simple form scalar differential delay equations still remain open in general case.

IVANOVIĆ, Dečan (Mechanical Engineering Department, University of Montenegro, Podgorica, Yugoslavia)

Unsteady boundary layer of incompressible fluid flow on aerofoil

The boundary layer equations are transformed into generalized form by introducing the appropriate variable transformations, momentum and energy equations, and a set of similarity parameters. Numerical integration of these equations with boundary conditions has been performed by means of finite difference method and Tridiagonal Algorithm Method with iterations, in the full two-parameter approximations with respect to the unsteady and dynamic parameter and their derivatives. Universal solutions are used to calculate the characteristic properties (skin friction, momentum and displacement thickness), if nondimensional potential external velocity is measured in free flight. It was found that the separation point moves along the aerofoil for accelerating fluid flow, and it moves toward the stagnation point for decelerating flow.

IWASAKI, Yoshimitsu (Okayama University of Science, Faculty of Informatics, Japan)

Physico-mathematical interpretation of the multiple anelastic relaxation in solids

Based on an axiomatic theory of the multiple anelastic relaxation in solids, a general linear ordinary differential equation of two infinitely differentiable functions, say, stress and strain, is introduced as a defining equation of the general linear solid. A diffusion operator corresponding to the Voigt solid in the mechanical model plays an important role to factorize the differential equation in the form of a product of diffusion operators as a result of an algebraic treatment. Natural correspondence of mathematical properties to physical properties of the general linear solid is further discussed.

IWASHITA, Takeshi (Department of Electrical Engineering, Kyoto University, Japan)

Parallel finite element electromagnetic field analysis of moving materials

Parallelized finite element analysis is carried out for a 3-D eddy current problem with moving materials. First order brick edge elements are used. In this moving material problem, it is important to solve fast the large scale sparse linear systems because many iterative computations are performed for the transient analysis. Parallelized solvers are introduced for solving the linear system. The analysis shows that a hybrid of the parallelized incomplete Cholesky preconditioning with substructure concept and the parallelized CG method can solve efficiently the linear system. This is a joint work with Masaaki Shimasaki.

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JALICS, Miklos (Ohio State University, USA)

Steady crystal growth in long ampoules in a vertical Bridgman device

One purpose in studying the steady growth of a crystal in a vertical Bridgman is the hope of determining optimal conditions for preparing crystals of high quality. I investigate how long an ampoule must be for steady crystal growth by solving the heat transfer in a long ampoule through numerical techniques. I use a combination of algebraic mappings, finite difference approximations, Newton's method, and preconditioned GMRES. Results show that the ampoule length must scale with the inverse of the square root of the sidewall Biot number. This is a joint work with Greg Baker and Mark Kunka.

JANNO, Jaan (Institute of Cybernetics at Tallinn TU, Estonia)

Lavrent'ev regularization of nonlinear ill-posed problems

Lavrent'ev regularization of nonlinear ill-posed operator equations in Hilbert spaces endowed with scales of inner products is considered. It is proved that the convergence rate of the method is $\sqrt{\delta}$ provided the Frechet derivative of the operator is Lipschitz-continuous and accretive and the exact solution is source-representable.

The theory is applicable to nonlinear Volterra equations of the first kind, particularly to the autoconvolution equation.

JELEN, Jaroslaw A (NOVA Research & Technology Co, Canada)

Non-iterative solution of Navier-Stokes equations

The compact methods are high accuracy finite difference methods where the functions and their derivatives are considered to be unknown. They originated from the rational-fraction or Padé differencing approximations. The compact schemes present the advantage over classical higher order methods by using a smaller stencil and yet resulting in smaller derivative discretisation error. This paper report on a novel numerical solution method for the incompressible Navier-Stokes equations. The proposed approach is based on a general compact method. General, in the sense, that it relates the values of a differential operator at stencil points to the values of the function at these points: (*) $\sum_{\nu} \alpha_{\nu} \mathcal{L}(u)_{\nu} = \sum_{\nu} a_{\nu} u_{\nu}$; whereas, the classical approach deals only with each of the derivatives separately. Weighting coefficients α_{ν} and a_{ν} are determined using Taylor series expansions. We extended (*) to handle a non-linear differential operator \mathcal{P} and constructed a non-linear version of scheme (*): $\sum_{\nu} \alpha_{\nu} \mathcal{P}(v)_{\nu} = \sum_{\nu} P(v)_{\nu}$. Although the concept can be extended to a wide range of non-linear problems with polynomial type non-linearities, the incompressible Navier-Stokes equations will be used here to illustrate the proposed non-iterative direct solution method.

JOHNSTON, Clifton Reed (University of Calgary, Canada)

Solitary wave solution for axially and radially deforming arteries

Nonlinear solitary waves are investigated by direct analysis of the field equations for blood flow in arteries. Axial and radial deformation of the artery are considered in the derivation of the field equations. The amplitude, speed and shape of the solitary wave are determined and compared to the case where axial deformation is neglected, therefore establishing the magnitude of the error resulting from neglecting arterial axial deformation.

KAKO, Takashi (The University of Electro-Communications, Japan)

On the stability of Newmark's method for the second order equation with general dissipation term and its application to resistive MHD problem

For the second order time evolution equation with a general dissipation term, we consider the stability condition for Newmark's method. We treat the case with a dissipation term satisfying the assumption that a damping matrix is constant in time and nonnegative. We don't need the assumption of the Rayleigh damping. We give the proofs of stability and convergence of the scheme by an energy method. We apply the results to a model resistive MHD equation.

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KALMÁR-NAGY, Tamás (Cornell University, Ithaca, USA)

Delay oscillators with high frequency excitation

Prediction of vibrations in material removal processes such as cutting and drilling is obviously important. Some of these vibrations arise due to a regenerative effect. Regenerative effects occur when the marks left by the tool on the workpiece affect future motion of the tool. The mathematical model describing these kind of processes is a delay-differential equation. Experiments as well as numerical and theoretical results showed the existence of periodic, quasiperiodic motions and even chaos in these models. Another possible source for tool vibration is the excitation of the tool caused by periodic chip formation. Chip formation is caused by an elastoplastic thermal instability called 'shear banding'. This high frequency process also affects the tool dynamics. The aim of the paper is to explore the effects of coupling between the microscale (chip segmentation) and macroscale (tool motion) dynamics. This is a joint work with Francis C Moon.

KALPAKIDES, Vassilios K (Department of Mathematics, University of Ioannina, Greece)

On the symmetries of non-linear thermoelasticity

The symmetries of the system of partial differential equations governing one-dimensional, non-linear thermoelasticity are studied by a method coming from exterior calculus. The infinitesimal generators of the transformations group and the similarity solutions associated with the system are derived. The admissible set of energy function for the problem under study, is produced and the reduction of the problem to a system of ordinary differential equations is presented. Also, the particular case of homogeneous thermoelastic materials is studied and the Lie algebra generated by the group of infinitesimal transformations is presented.

KAMITANI, Atsushi (Faculty of Engineering, Yamagata University, Japan)

Magnetic shielding performance of HTS plates with arbitrary cross section

The magnetic shielding performance of the high-Tc superconducting (HTS) plate with an arbitrary cross section is numerically investigated by use of the flux-flow-creep model. By taking account of the crystallographic anisotropy of the HTS plate, the HTS plate is assumed to have a multiple thin-layer structure. Under these assumptions, the governing equations of the shielding current density can be expressed in terms of a scalar function. The numerical code to integrate the equation has been developed and, by use of the code, the damping coefficients are calculated as functions of time and the frequency of the applied magnetic field. This is a joint work with Takafumi Yokono and Shigetoshi Ohshima.

KANAYAMA, Hiroshi (Kyushu University, Japan)

A finite element approach for 3-D eddy current problems

A method for 3-D eddy current analysis of an asymmetrical conductor with a hole (Problem 7 in TEAM Workshop) was given in ICES'95 and ICES'97. Adopting the ALE formulation, we approximated a weak formulation by the mixed finite element method which was originally developed by the second author (F. KIKUCHI, The University of Tokyo) for the magnetostatic analysis. Before this method, we tried another approach adopting the H-J formulation. However, because of some difficulties, we changed the approach. In this paper, some considerations are added for this problem and some numerical results by the H-J formulation are demonstrated for the first time. Also, some solvers for the resultant large sparse non-symmetric linear equations are discussed.

KANEKO, Akihiko (University of Tokyo, Japan)

On a non-linear modelling analysis for complex time series

As an application of the local theory for non-linear information analysis, we develop a non-linear modeling analysis for local stochastic processes and pursue a non-linear modeling and prediction analysis for some concrete complex time series in natural phenomena, life phenomena, technological phenomena and social phenomena. This is a joint work with Yasunori Okabe.

KASYANOV, Victor N (Institute of Informatics Systems, Russia)

Support tools for supercomputing

The project PROGRESS being under development at the Institute of Informatics Systems in Novosibirsk is discussed. The system is intended to support rapid prototyping of compilers for high level languages (e.g. Fortran-77, Modula-2, Sisal-90) and for a family of architectures exploited fine-grained parallelism. The next goal of the project is to develop an environment for investigation of optimizing and restructuring transformations of programs to be parallelized. The information subsystem TRANSFORM aimed at accumulating and processing of knowledge about optimizing and restructuring program transformations is considered. The subsystem SFP intended to supporting numeric high-performance computation on the base of the applicative language Sisal-90 is outlined. The work is supported by the RFBR under Grant 98-01-00748. This is a joint work with V A Evstigneev, J V Malinina, J V Birjukova, V A Markin, E V Haritonov and S G Tsikoza.

KAWAMURA, Takeshi (Kitami Institute of Technology, Japan)

Γ -stability analysis with monotonicity conditions

We will present the Γ -stability analysis of the characteristic polynomial whose coefficients are polynomials of interval parameters. The Γ -stability conditions are studied mainly on the expansion of the boundary crossing theorem by J. Ackermann, et al. Most condition need calculation on the whole parameter region. Under the assumption of the monotonicity with respect to the interval parameters, we derive the necessary and sufficient conditions of the Γ -stability using only the endpoints of interval parameters. The monotonicity conditions are also checked by our monotonicity test at the endpoints of interval parameters. This is a joint work with M Shima.

KAY, Anthony (Loughborough University, UK)

Finite-time blow-up in an inviscid buoyancy-driven flow

Matched asymptotic expansions are used to examine the approach to blow-up of an inviscid flow driven by a horizontally quadratic density gradient and confined between horizontal plates. The flow and density gradient intensify in an inner region near one of the plates; the thickness of this region decreases as $-\frac{1}{\ln \tau}$ where τ is the time remaining until blow-up. Uniform expansions are found for the flow in this region together with the outer region, but the influence of initial conditions persists in a non-uniform region near the opposite plate. In a rotating frame blow-up is delayed, and may proceed by the growth of inertial oscillations. This is a joint work with R E Grundy, University of St Andrews, UK.

KERN, Michel (INRIA France)

Using Gröbner bases to compute higher order finite elements for mass lumping

Finite element solution of the wave equation allows easy handling of complex geometrical features, such as topology for geophysical modeling. Retaining higher order accuracy while remaining explicit requires a diagonal mass matrix, so the finite element must have a built-in quadrature formula of sufficiently high order. Constructing such a finite element leads to the solution of a system of polynomial equations for the values of the quadrature nodes and weights. Applying symbolic algebra techniques enables us to obtain exactly the number of real positive solutions, as well as obtaining approximate values. We describe how techniques from the Gb and RealSolving toolboxes help solve this problem. This is joint work with Jean-Charles Faugère (LIP6), Frédéric Hannyoy, Agany Oloui and Fabrice Rouillier.

KERR, Gilbert (New Mexico Tech, USA)

An effective numerical algorithm for the annular crack problem

In this paper we determine the stress intensity factors for an annular crack in an isotropic solid, subjected to a prescribed load. The problem is formulated, such that it reduces to that of solving one singular integral equation. A numerical algorithm for solving this equation is then developed and the stress intensity factors are computed directly from its solution. The results obtained are in exact agreement with those found in several previous publications. The new algorithm, however, requires significantly less computational effort than any of its predecessors

KEYES, David E (Old Dominion University and ICASE (NASA Langley Res. Ctr.), USA)

Parallel implicit methods for CFD and diffusive radiation transport

For coupled PDE systems from aerodynamics and radiation transport we employ iterative algorithms of Newton-Krylov-Schwarz (NKS) type on distributed-memory architectures consisting of thousands of processors, and study three aspects of performance: (1) the trade-off of convergence rate with cost-per-iteration as preconditioner quality and global synchronization frequency are varied, (2) parallel scalability, and (3) fraction of peak flop/s that can be captured. NKS methods prove broadly applicable and tunable for high efficiency on today's high-end platforms for structured and unstructured computations. However, with an increasing premium on latency tolerance, we document needs for increased expressiveness in scheduling and data placement, and therefore new algorithm designer responsibilities.

KEYFITZ, Barbara L (University of Houston, USA)

Transonic shocks in steady and quasisteady flows

In studying two-dimensional Riemann problems for conservation laws, we find that the principal challenge is understanding the flow in the subsonic region, where the governing equation is degenerate elliptic (for simplified models such as the unsteady transonic small disturbance equation or nonlinear wave equation) or even of mixed type. In joint work with Sunčica Čanić, we have made progress on two fronts: we have obtained existence and regularity results for prototype problems involving degenerate elliptic equations such as occur in self-similar reductions of conservation laws. Also, in joint work with Gary Lieberman, we proved a related result for transonic shocks in the steady transonic small disturbance equation. We prove that for any sufficiently small upstream perturbation, there exist a steady perturbed shock, satisfying the Rankine-Hugoniot conditions, and a continuously differentiable solution, which remains close to the uniform solution, in any bounded region downstream. The downstream flow, augmented by the Rankine-Hugoniot conditions, is the solution of a free boundary problem. The talk will report on these developments.

KHAN, Winston (UPR-Mayaguez, Puerto Rico, USA)

Extension of Danckwert's surface renewal theory to all interfacial conditions

Danckwert's propounded his surface renewal theory for interfacial turbulent mixing in transport phenomena that occurs in engineering problems. He envisaged that eddies were impelled into the interface from the bulk phase in stirred systems.

KHENTOV, Anatoli A (Nizhni Novgorod State University, N Novgorod, Russia)

Resonance regimes in the dynamical systems and the peculiarities of motions for Jupiter's and Saturn's satellites

A theory of quasi-stationary resonance solutions for the systems differential equations with fast rotating phases in the critical cases was created. The theorems about conditions of the existence and stability for these solutions were proved. The extremal criterions of a selection for the stable resonance motions of the celestial bodies were received on a base of these theorems. The exact necessary conditions were obtained for the stability of resonance orbital motions in classical problem of many celestial bodies with mean angular velocities related by several resonance relations. The explanations of wonderful phenomena in the orbital motions some Jupiter's and Saturn's satellites were suggested.

KILPATRICK, Peter L (The Queen's University of Belfast, UK)

Specification of a complex scientific domain using a formal notation

The OpenMol project addresses the development of software solutions to problems in certain characteristic domains of quantum chemistry. This paper focuses on the intelligence aspect of OpenMol: providing computer-aided expert guidance for the solution of problems. The technique employed is Case-based Reasoning whereby one uses a case base of existing problems and their solutions as the basis with which to solve new problems. Essential to the construction of such a case base is a precise specification of the domain of interest. The development of such a specification using the formal specification notation VDM-SL is described. VDM-SL is based on set theory and the predicate calculus. This is a joint work with G H F Dierksen and E W Schreiner Max-Planck-Institut für Physik. Germany.

KIM, Hyeock-Jin (Chungwoon Univ, Korea)

Data exchange by the degree reduction of B-splines

The data exchanges for the curves and surfaces between the different geometric modelings need the degree reductions on approximating to the degree of supporting system within given tolerance, when the maximum degree of the supporting system is less than that of inputs. We have studied on a data exchange on B-splines degree reduction and proposed a method to reduce the degree of B-splines. Our approximate curves are implemented and compared experimentally with the others from the different degree reductions of Bézier curves. It has been also possible to find that ours are more desirable. This is a joint work with Dr. & Prof. Ha-Jine KIMN, Ajou University, Korea.

KIM, Mi-Young (Dept of Math, Yonsei University, Seoul, Korea)

Characteristic Galerkin finite element methods for diffusion epidemic models

A numerical approximation is considered for a model of epidemiology describing age-dependent population dynamics with spatial diffusion. A finite difference method along the characteristic age-time direction is combined with finite elements in the spatial variable. Long time behavior of the discrete solution is also investigated. Optimal order error estimates are derived for the approximation.

KIMURA, Hiroshi (University of Tokyo, Japan)

Multifractal analyses of the derived measures on FM method

A fractal multifractal (FM) method is one of the fractal geometrical approaches which is introduced by C. E. Puente. In this method, complex measures are derived using multifractals and self-affine fractals and these derived measures are useful to model complex hydrologic phenomena. However, relations between FM parameters and the derived measures are not clear. Therefore, in this research, the relations are analyzed using generalized fractal dimensions D_q of the derived measures.

KIRKEGAARD, Peter (Risø National Laboratory, Roskilde, Denmark)

Numerical simulation of chemical reaction systems: CHEMSIMUL

CHEMSIMUL is a computer program system for modelling complex kinetics in atmospheric chemistry, combustion processes, photochemistry, and radiation chemistry. It contains a translator module, a mass balance test module, and a module for solving the resulting coupled nonlinear ordinary differential equations. Algebraic "plot expressions" are processed by maintaining stacks of operands and operators. An overview of these features and their interplay is given. Moreover we describe a new stoichiometric mass balance algorithm based on linear programming. The use of the system is illustrated by examples. This is a joint work with Erling Bjergbakke, Risø National Laboratory, Denmark.

KOHNO, Toshiyuki (Okayama Univ. of Science, Japan)

On the generalized modified Gauss-Seidel method

We extend the modified Gauss-Seidel method. This method is preconditioned iterative method which uses a preconditioner $(I + S_{max})$ derived from A . S_{max} is composed of the biggest element at each row of the upper triangular part of A . Some numerical examples show that our method is able to improve the rate of convergence compared the modified Gauss-Seidel method.

KOLLMANN, Wolfgang (MAME, University of California Davis, USA)

Hybrid spectral-finite difference Navier-Stokes solver for spatially developing incompressible flows

An accurate solution method for the 3-d, unsteady, incompressible Navier-Stokes system suitable for DNS/LES of round jets, wakes and pipe flows is developed using cylindrical coordinates. The azimuthal spatial direction is treated spectrally using Fourier collocation and the other directions are discretized using high order finite difference methods. Time integration is done with a third order Williamson type (see Williamson, J.H. (1980), *Low-storage Runge-Kutta schemes*, J. Comput. Phys. **35**, 48-56) Runge-Kutta method. The equations in cylindrical coordinates are more complicated than their Cartesian counterparts and the coordinate axis $r = 0$ requires careful analysis to take full advantage of the periodicity in azimuthal direction. The results of this analysis show that the azimuthal Fourier modes of scalars, vectors and tensors possess distinct symmetry properties with respect to the radial direction and satisfy growth laws dependent on the azimuthal wavenumber. Mass balance is eliminated using complex-valued streamfunctions associated with the azimuthal Fourier modes of velocity. The streamfunctions satisfy Poisson equations, which are solved using either a LU-decomposition method or a full multi-grid solver. The resulting method is verified for several vortical flows at Reynolds numbers ranging from 2000 to 5000. These include vortex breakdown in a pipe with rotating endwall (see Escudier, M.P. (1984), *Observations of the flow produced in a cylindrical container by a rotating endwall*, Experiments in Fluids **2**, 189-196), vortex pinch-off (see Gharib, M., Rambod, E. and Shariff, K. (1998), *A universal time scale for vortex ring formation*, JFM **360**, 121-140) and round jet.

This is a joint work with J Y Roy, MAE Dept., University of California.

KONTOROVICH, Valeri Ya (CINVESTAV-IPN Mexico)

Envelope and phase for narrow-band random processes with jumps.

In this paper the Markovian features of the envelope and phase for narrow-band processes with jumps are considered. Such processes are generated by the stochastic differential equation of the second order (SDE-II) excited by Poisson successions of d-pulses with random "amplitudes". For this matter a special type of the Kolmogorov-Feller integro-differential equation was developed and it is shown that Markovian properties of the envelope and phase depend on the Poisson excitation intensity and narrow-band features of the dynamic system for SDE-II. Special cases of "high" and "low" intensities of d-pulse Poisson successions were investigated as well.

KOROBENIKOV, Victor P (Institute for Computer-Aided Design, Russian Academy of Sciences, Moscow, Russia)

Analysis of critical states of physical systems by catastrophe theory

Using mathematical catastrophe theory, we study the behaviour of different physical systems near their critical states. The critical state is a fast alteration of the system state under the continuous changing of the main parameters. Here we study the cases of ignition and extinction of flame, electric breakdown, phase transition and similar phenomena. The dynamical systems of ODE and PDE systems of diffusion type are used in the study. Values of basic variables for the critical states (temperature, density, electric field intensity, etc) are determined and the systems behavior near these states are investigated. This is a joint work with D.Vorobiev.

KORZEN, Manfred (Bundesanstalt fuer Materialforschung -und pruefung (BAM), Fire Engineering, Berlin, Germany)

Fast data assimilation in fire tests of steel members

The proposed method is used to produce an interpolating time and space temperature distribution for steel members subject to fire testing. The physical model is derived from the non-linear, transient heat equation $c_v \rho \partial_t u = \nabla(k \nabla u) + J$, which is discretized on a finite difference grid and solved iteratively in time for u_j^n with a data assimilation step at each iteration, i.e. (1) Given at time t_n are the values u_j^n on the fine grid x_j and the collected data as u_j^{n+1} on the thermocouple grid x_j . (2) Using the collected data u_j^{n+1} at time t_{n+1} , solve (1) for J_j^n on the coarse grid. (3) Interpolate J_j^n to the fine grid by a method, which depends on the ansatz for $J(u, x, t)$. (4) Solve (1) for u_j^{n+1} on the fine grid to get the temperature distribution at time t_{n+1} . (5) Set $n \rightarrow n + 1$ and go to step 1.

KOSTINA, Ekaterina (IWR, University of Heidelberg, Germany)

Robust parameter estimation for dynamic systems

The traditional method to determine unknown parameters in DAE model is by the least squares (l_2) technique. When the measurement data is good (without "outliers") this method proved to be appropriate. When the measurement data is bad (in the presence of "outliers") the use of l_1 technique is recommended since the solution obtained by this technique is insensitive (robust) to "outliers". The talk deals with the algorithm of robust parameter estimation for dynamic systems which combines the boundary value approach and a special method of solving l_1 approximation problem. The method is successfully applied to several real-life problems.

KOVTUN, Irina I (National Agricultural University, Kiev, Ukraine)

The systems of differential equations with non-Gaussian stochastic perturbations

We investigate the systems of differential equations with stochastic perturbations. For finding the probability characteristics of the solutions of such systems, we obtain certain closed integro-differential equations. In the case of Gaussian perturbations, the moment equations are simplified and reduced to differential ones. The results are applied to investigation and synthesis of the drive mechanism of working organs of multifunctional mobile machines under stochastic perturbations.

KOZIEN, Marek S (Cracow University of Technology, Poland)

Influence of the angle of coupling on vibrational energy transmission for the jointed plate-like elements

There are several papers and books which deal with a problem of influence of the angle of coupling on the vibrational energy transmission for the jointed continuous elements as rods, plates or shells. Most of them present results of analyses done for geometrically semi-infinite structures. The realistic engineering structures are built however of the finite dimensioned ones. Some dynamical effects for that two kinds of structures are completely different indeed (e.g. travelling waves - standing waves, eigenforms, boundary conditions). This is the reason of making analyses for finite structures. The author estimates the influence of the angle of coupling for the jointed plate and cylindrical shallow shell elements. The analysis was done by application of the finite element computer package NISA II. The analysis was done for the low modes. The results of analysis show the possibility of reducing the amplitudes of vibrations of chosen element by changing the value of the angle of coupling. It is a very important way for the case of structures built in part of glasses e.g. cages of heavy duty machines. It was shown before that vibrations of glasses are the source of the noise inside cages. This work was sponsored by Polish National Research Committee under the grant no. 7T07B 009 15.

KOZYREVA, Ekaterina (1, 1st Dorozhny pr., Moscow 113545, Russia)

Elastic rod model of 3D structure of RNA

A problem of reconstruction of approximate large-scale 3D structure of an RNA molecule from its secondary structure is considered. Both a new mathematical model and its computer implementation are presented. An RNA molecule is treated as a set of basic structural elements (stems and loops of various type) modelled by elastic rods. A numerical procedure is developed for computation of shapes of the RNA elements and for assembling the whole molecule. The comparison of the available X-ray diffraction analysis results (yeast phenylalanine tRNA) with the proposed rod model reveals a good correspondence of the overall tracing of the polynucleotide chain. This is joint work with E.I. Kugushev and Eugene L Starostin.

KREJIĆ, Nataša (Institute of Mathematics, University of Novi Sad, Yugoslavia)

A Newton-like method with modification of right-hand side vector

This paper proposes a new Newton-like method which defines new iterates using linear system with the same coefficient matrix in each iterate, while the correction is performed on the right-hand side vector of the Newton system. In this way a method is obtained which is less costly than Newton method and faster than fixed Newton method. Local convergence is proved for smooth mappings. The influence of the relaxation parameter is analysed and explicit formulae for the selection of optimal parameter are presented. Relevant numerical examples are used to demonstrate the advantages of the proposed method.

KRIVONozhko, Vladimir Egorovich (Institute For Systems Analysis, Russia)

The optimization models to efficiency analysis of the complex systems

The current tense financial situation in Russia makes companies increase their efficiency. We propose new approaches within DEA framework to determine the efficiency of complex production systems. We calculate the stability regions and determine critical and optimal directions for every investigated DMU. The preferable targets are chosen and the optimal paths are found to reach these targets. We propose an approach that allows us to replace the solution of large-scale DEA problem by the solution of a relative small problem. Applications of the approaches to the analysis of the 35 leading Russian oil companies and 150 banks will be shown. This is joint work with Oleg B Utkin and Roman Vic Senjkov.

KRIVTSOV, Anton (University of Aberdeen, King's College, Aberdeen, UK)

Influence of nonconservative forces on stability of high speed drilling

Modern mechanisms used for rotary machining are exposed to very high speeds, which can cause serious stability problems due to the reaction forces and moments occurring during the cutting process. In the paper it is shown that nonconservative moment evoked by contact of the drilling tool with the material can induce instability of the rotor if 3D dynamics of the system is taken into account. Different models for the cutting processes are examined. Conditions of stability are obtained. Application to ultrasonically enhanced drilling process is also considered. This is a joint work with M Wiercigroch.

KUBENKO, Veniamin D (Institute of Mechanics of National Academy of Sciences, Ukraine)

Dynamics of the spherical inclusions in the endless cylindrical vessel containing flowing liquid

The problem is solved dealing with interaction of infinite circular cylindrical vessel (shell) containing flowing ideal incompressible liquid and a vibrating spherical inclusions (particles, bubbles or their family) in it. Only small amplitudes of vibrations are considered, therefore a linear theory of elastic shells is used and behavior of liquid is described by Laplace or Helmholtz equation for the incompressibility or compressibility of it, respectively. The undisturbed liquid can be in rest or in axial motion. Approach to the solution of such problem is based on re-expansion of partial solutions of the Laplace's equation written in the cylindrical (spherical) coordinates by the spherical (cylindrical) harmonic functions respectively. Satisfaction of the boundary conditions on the cylindrical and spherical surfaces permits to reduce the solution of the problem on the research of the desired potential to the solution of the infinite system of linear algebraic equations. The concrete numerical results are presented. The obtained results may be used for modelling and researching processes concerning with stream of the physiological liquids in the vessels. A case of viscous liquid is discussed as well.

This is a joint work with Lesia Kruk.

KUBOTA, Koichi (Dept. Information and System Engineering, Chuo University, Tokyo, Japan)

A preprocessor for reverse automatic differentiation with recursive checkpointing

Given a program computing the value of a function with many variables, the reverse mode automatic differentiation swiftly computes the values of the gradient. However, it requires storage whose size is proportional to the complexity of the underlying function. We report on a Fortran77 preprocessor for the improved reverse mode automatic differentiation with the recursive checkpointing mechanism. Using the fork system-call on the UNIX operating system, we developed a library named RCL/fork (Recursive Checkpointing Library with fork system-call), and we could drastically reduce the size of the virtual memory.

KUMAGAI, Teruo (Science University of Tokyo, Japan)

Reevaluation of Oseen's approximation for prediction of rotating motions of a cluster of spheres in fluid at low Reynolds numbers

Free-fall motions of micron-order particles in nature or industrial applications are classified into the Stokes-range motion at Re below 0.1 and the Oseen-range motion at Re between 0.1 and 1.0. A new method for the Oseen-range motion is proposed to estimate the hydrodynamic interaction among the particles by superposing the Oseen's flow field as the 1st approximation to the reflection method, which is a kind of asymptotic method. This superposition method predicts newly-recognized diffusive and rotating motions of a cluster of spheres.

KUTZ, J Nathan (Department of Applied Mathematics, University of Washington, USA)

Dynamics, bifurcations, and stability of fronts in the optical parametric oscillator

We consider the dynamics, stability and bifurcation of front structures of the optical parametric oscillator. Front solutions bifurcate super-critically from the trivial solution to a neutrally stable, translationally invariant front. Perturbations such as white-noise, group-velocity walk-off, or non-uniform pumping simply shift the center position of the front solution. For 2D fronts, the front curvature is governed by the heat equation so that only stripes are supported for long times.

This is a joint work with T Erneux, Universite Libre de Bruxelles, Belgium.

KUZMINA, Lyudmila K (Kazan Aviation Institute, Russia)

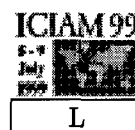
Models and methods in dynamics of complex systems

The paper is concerned the different aspects of mathematical modelling and analysis in dynamics of complex non-linear systems, that are generated by applied problems of engineering practice. Main aims are the problems of optimal (in some sense) mechanical- mathematical modelling and the regular schemes of decomposition in Engineering Design and Automation. Here uniform methodology, based on Lyapunov's methods, in accordance with Chetayev's stability postulate, is developed. The presented approach allows to elaborate the general conception of the modelling; to work out the simple schemes of engineering level for decomposition of full systems and dynamical properties.

KWAK, Do Y (Korea Advanced Inst. Sci. Tech(KAIST), Korea)

Extraordinary convergence of multigrid method for triangular grid

In this paper, we prove a V -cycle convergence of a multigrid method for the mean value solution of a Helmholtz equation using triangular grid. The convergence is faster than the standard model problem on the unit square using P_0 finite element.



LAI, Choi-Hong (University of Greenwich, UK)

An acoustic expansion method for the retrieval of noise signals in unsteady flow

This paper proposes a strategy, based on the concept of defect corrections, for the retrieval of noise signals. The full physical quantities such as pressure and velocities may be fully expanded by retrieving the acoustic perturbation from the defect equation. This paper examines ways of calculating residuals accurately, meshes used for the defect equation and the numerical methods for solving the defect equation. Numerical tests for vortices of variable strength impinging on an aerofoil are presented.

This is a joint work with G S Djambazov and K A Pericleous.

LAZAREV, Alexander A (Kazan State University, Russia)

Analyze of structure of optimal schedule the problem minimizing maximum lateness for single machine

We study NP-hard problem of theory of scheduling $1 \parallel \sum T_j$. The jobs of set N have integer processing times p_j and due dates d_j . Were constructed pseudopolynomial algorithm complexity $O(n \sum p_j)$ time and polynomial algorithm $O(n^2)$ time. Was finded structure of optimal schedule.

LE BRIZAUT, Jean-Sebastien (ECN, BP, Nantes Cedex, France)

A solution of mixed partial differential equations

The aim of this communication is a numerical method to solve nonlinear partial differential equations of mixed type. The solution consists in minimizing a functional - the number of variables corresponds with the number of the discretization points. It proceeds from the following scheme: computation of the solution using a minimization with a quite large discretization, interpolation of the result in order to obtain the initialization of the last step, computation of the solution using a minimization method with a more precise discretization. The tests are performed with an explicit example to warrant the validation of the numerical results. This is a joint work with Marc Pogu.

LI, Lei (Faculty of Science, Yamaguchi University, Yamaguchi, Japan)

Fast parallel algorithms for Vandermonde determinants

We know that evaluating an $n \times n$ Vandermonde determinant usually needs $O(n^2)$ number of arithmetic operations. This paper presents a few fast algorithms for Vandermonde determinants, confluent Vandermonde determinants and generalized Vandermonde determinants. These algorithms need only $O(n \log_2^2 n)$ number of arithmetic operations on a serial computer, or at most need $O(\log_2^2 n)$ number of the parallel steps on a SIMD type supercomputer with n processors.

LI, Qian (Yamagata University, Japan)

A factoring algorithm using quadratic residue

The problem of finding the prime factors of large composite numbers has always been of mathematical interest. With the advance of public key cryptosystems it is also of practical importance, because the security of some of these cryptosystems, such as the Rivest-Shamir-Adelman (RSA) encryption scheme, the RSA signature scheme, and the Rabin encryption scheme, depends upon the intractability of the integer factorization problem.

In this report, we do a study upon an integer factoring algorithm based on new idea that using quadratic residue. This method is effective especially on factoring Blum numbers and on $n = p^2q$ type composite numbers.

LI, Shidong (San Francisco State University, USA)

Subspace signal expansions with off-the-space sequences and applications

We introduce a notion of series expansions of a subspace \mathcal{X} with sequences of functions not necessarily contained in \mathcal{X} . We call them *pseudoframes for subspaces* (PFFS). Our study of PFFSs are motivated by examples from the classical sampling theorem and by problems in signal processing. Series expansions with PFFSs have greater flexibility that are attractive (particularly) in applications. Properties of PFFSs will be discussed. A necessary and sufficient characterization of PFFSs will be provided. Analytical formulae for the construction of PFFSs shall also be given. Examples and applications of PFFSs to a robust irregular sampling formulation will be discussed in detail.

LI, Tong (Department of Mathematics, University of Iowa, Iowa City, USA)
Global bv solutions and relaxation limit for a traffic flow model

We construct global solutions and study their large-time behavior for a system of nonlinear hyperbolic conservation laws with relaxation arising in traffic flows. The system was derived as a continuum model of traffic flows. The main innovation of the system is that it addresses the anisotropic feature of traffic flows so there is no 'wrong-way travel', as presented in other models. As a direct consequence of the anisotropic feature of traffic flows, the hyperbolic system with relaxation is degenerate in the sense that the subcharacteristic conditions are not satisfied. Thus the existing theory based on Chapman-Enskog expansion does not apply. Our analysis is based on a generalized Glimm scheme and the relaxation nature of the problem.

LIMAYE, Balmohan V (Indian Institute of Technology Bombay, India)

Accelerated refinement of approximate eigenlements of integral operators

A new approach based on the framework of a product space, is presented for constructing iterative schemes for refining approximate eigenlements of integral operators. A polynomial eigenvalue problem is lifted to an equivalent linear eigenvalue problem in a product space, where the iterates achieve geometric rates of convergence, while the size of the problem is increased only arithmetically. In the product space formulation, the schemes depend on a positive integer q which specifies the desired rate of convergence and it equals the the number of copies of the original space taken in defining the product. The approach is illustrated by considering a Newton type refinement scheme for a simple eigenvalue and a corresponding eigenvector of an integral operator. This is a joint work with R Alam and R P Kulkarni.

LIN, Feng Lee (Department of Business Management, National Sun Yat-Sen University, Taiwan)

Modeling a reliability location problem by Taguchi's approach

An integer programming is often applied to solve a reliability location problem, however, the solution may varies with its parameters and the computation complexity may blow up if its size increases. Instead of conducting a post-optimality analysis, the Taguchi's approach is applied to model a reliability location problem so that a robust solution can be obtained quickly. The model uses the "noise" intervals of the parameter values as input and provides an interval solution rather than a point solution. An example of telecommunication is adopted to demonstrate the use of the proposed method.

LIN, Jen-Jen (Dept. of Statistics, Ming Chuan University, Taipei, Taiwan)

A new algorithm of independent component analysis with application

This study is to propose a new algorithm of independent component analysis (ICA) to transform a set of dependent random variables into independent normal random variables. An obvious advantage of deriving independent components is that we can sample the correlated multivariate variables by sampling the univariate independent variables. Joint multi-normality will be assessed by the empirical P-value of the tests based on generalized Shapiro-Wilk (SW), Cramer-Von Mises (CVM) and the Kolmogorov Smirnov (KS) statistics. Multivariate skewness and multivariate kurtosis are also calculated. For independency, we will, under the assumption of multi-normality, check if the covariance matrix is diagonal. Possible applications of the algorithm are discussed and some numerical results are presented. This is a joint work with Naoki Saito, Dept. of Math., University of California, USA and Richard A Levine, Div. of Stat., University of California, USA.

LOZIER, Daniel W (National Institute of Standards and Technology, USA)

The DLMF project: a new initiative in special functions

The Handbook of Mathematical Functions (Abramowitz and Stegun, Eds., 1964) remains a universal reference among physical scientists, engineers, mathematicians and statisticians, according to analyses of Science Citation Index, but this distinction is increasingly jeopardized by decades of advances in mathematics and computing. Also, because of rapidly developing Internet capabilities, an unprecedented opportunity exists to construct a computerized database and powerful tools to help users locate, retrieve, visualize and interact with authoritative, up-to-date information on special functions. Recent progress of a NIST initiative to achieve this goal will be discussed. This is a joint work with F W J Olver, Maryland, C W Clark, NIST and R F Boisvert, NIST.

LU, Kai-Sheng (Wuhan Transportation University, China)

Structural conditions of controllability & observability over $F(Z)$ for RLC networks

Let all physical parameters (resistors, inductors and capacitors) of an RLC network be independently variable parameters. The network is then called one over the field $F(z)$ of rational functions in the parameters. The speaker presents two structural conditions: 1. If an RLC network without sources is unhinged and has no all-capacitor cut-sets or all-inductor loops, then the network is observable over $F(z)$ for any network variables (i.e., its node voltages and/or branch currents) as its output. 2. Assume that an RLC network has no all-voltage source-capacitor loops or all-current source-inductor cut-sets, and its network without sources has no all-capacitor cut-sets or all-inductor loops and is unhinged. Then, the network is controllable over $F(z)$ iff its sources and independent energy storage elements are unhinged. This is a joint work with Kunsheng Lu, Huazhong University of Science and Technology, China.

LU, Tzon-Tzer (Department of Applied Mathematics, National Sun Yat-sen University, Kaohsiung, Taiwan)

Inverses of 2×2 block matrices

We first give the explicit inverse formulae of 2×2 block matrix in three different partitions. Then we apply these results to get inverses of block triangular matrices and matrices with symmetry, including bisymmetric, Hamiltonian, perhermitian, and centrohermitian matrices, etc. Ascending algorithms computing the inverses of these matrices with symmetry follow. These results are also useful to solve the completion problems of 2×2 block matrix and its inverse.

LUDWIG, Bruno (AEROSPATIALE Centre Commun de Recherches, France)

Boundary integral equations for the problem of acoustic scattering by an absorbing obstacle

We consider the numerical resolution of acoustic scattering problem by an absorbing obstacle. It is well known that there are different methods to obtain boundary integral equations (BIE) permitting that numerical resolution. For the reduced wave equation, A. Bamberger and T. Ha-Duong proposed to use an interior problem corresponding to the same Robin boundary condition *with a change of sign on the impedance function*. That gives rise to a couple of BIE, with both the jumps of the acoustic pressure and velocity as variables. We present 3D numerical experiments that prove the efficiency of the method, and extend the idea to the case of time-dependent acoustic scattering problems. This is a joint work with Prof Ha Duong.

LUPU, Gheorghe (Ovidius University, Romania)

The hypergeometric function in the study of collision integral of the Boltzmann's equation

We have developed approximate and numerical methods to solve the Boltzmann's integro-differential equation. Here we present the calculus method for collision integral transformed by hypergeometrical functions. This is a joint work with C Grasu.

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MACKENS, Wolfgang (Technical University Hamburg-Harburg: Section of Mathematics, Germany)

Convergence analysis of Newton type couplings of subsystem solvers

Complex technical systems are often assembled from already existing components. The idea suggests itself to similarly synthesize numerical simulators of such systems from available simulators of subsystems. Such approaches facilitate utilising knowledge about the subsystems and spare the designer expensive re-validation of subsystem simulators. The coupling iteration for stationary problems that we will analyze assumes the subsystems to be accessible through iteration steps of their iterative solvers. Neither formulae nor source code have to be provided. We present techniques to achieve good local convergence of the total solution process and we address global convergence issues. This is a joint work with Juergen Menck and Heinrich Voss.

MAILYBAEV, Alexei A (Moscow State Lomonosov University, Russia)

On application of miniversal deformations to the stability theory

Miniversal deformations of complex matrices by Arnold (1971) and of real matrices by Galin (1972) give a powerful tool for studying different singularities and bifurcations in linear systems dependent on many parameters. However almost all applications of miniversal deformations lead to qualitative results, since the method of finding the transformation to the miniversal deformation has not been constructed yet. In the paper a recurrent procedure for finding transformation of a matrix family to miniversal deformation is suggested and applied to quantitative analysis of singularities of stability domain boundaries. Mechanical examples are given.

MARCHENKO, Nikolay A (Keldysh Institute for Applied Mathematics, Russia)

Structures of two-phase flow through double porosity media: numerical analysis

We consider the two-phase flow through a dual-porosity medium, characterized by a period of heterogeneity ε , a ratio of global permeabilities ω_K , and a ratio of the order of capillary forces ω_c . The classes of flows characterized with different values of ω_K and Peclet numbers Pe are investigated numerically. We used modified Niche method for solving the elliptic-parabolic system of PDE and difference scheme of flux correction for hyperbolic equations. The classification of flows is illustrated with results of 2D and 3D computer simulation. This is a joint work with M Panfilov, Oil & Gas Research In-te, A Kh Pergament, B D Plyushchenkov and V I Turchaninov, all - Keldysh In-te.

MARTEL, Carlos (ETSI Aeronáuticos, Universidad Politécnica de Madrid, Spain)

Parametrically forced counterpropagating waves in weakly dissipative systems

A system of two coupled complex nonlocal Ginzburg-Landau equations is considered. This system is the corresponding normal form for the weakly nonlinear evolution of a parametrically forced weakly dissipative system in a large annular domain. The nonlocal terms in the equations come from the fact that the two counterpropagating wavetrains that appear move in a very fast time scale as compared with the time scale in which dissipation, nonlinearity and dispersion come into play, and in this longer time scale each wavetrain feels only an averaged effect of the other. This is a joint work with J M Vega and E Knobloch.

MASON, David P (University of the Witwatersrand, Johannesburg, South Africa)

On the effect of interfacial tension on slow viscous flow past a spherical liquid drop

The interfacial tension required to maintain a spherical liquid drop in uniform, steady, slow viscous flow is investigated. Solutions for the stream function and the interfacial tension are derived to first order in the Reynolds number using matched asymptotic expansions. We find that, in an infinite expansion of Legendre polynomials, to first order in the Reynolds number the interfacial tension depends on Legendre polynomials only up to degree two. A stagnant fluid cap is found to exist inside the liquid drop at the rear. The interior and exterior flows are compared with slow viscous flow past a liquid drop with constant interfacial tension. This is a joint work with G M Moremedi.

MATSUURA, Masaya (University of Tokyo, Japan)

On a non-linear causal analysis for complex time series

As an application of the local theory for non-linear information analysis, we develop a non-linear causal analysis for two kinds of local stochastic processes and pursue a non-linear causal analysis for some concrete complex time series in natural phenomena, life phenomena, technological phenomena and social phenomena. This is a joint work with Yasunori Okabe.

MCKINLEY, Iain S (University of Strathclyde, Glasgow, UK)

Stability of a ridge subject to a jet of air

In this paper we consider the linear stability of a thin ridge of fluid on a planar substrate subject to a jet of air acting normally to the substrate. We investigate two cases: one in which the jet acts at the centre of the ridge and one in which the jet is off-centre. The results of our numerical calculations are described and the conclusions of our previous quasi-static analysis of this problem are reviewed in the light of these new results. This is a joint work with Dr S K Wilson and Dr B R Duffy, University of Strathclyde, Glasgow, UK.

MEHRI, Bahman (Department of Mathematical Sciences, Sharif University Of Technology, Tehran, Iran)

Numerical solution of Neumann problem for a nonlinear Poissons equation

The following boundary value problem is considered $\nabla u = u^\alpha$, $0 < \alpha < 1$, in D and $\frac{\partial u}{\partial n} = g$ on ∂D we shall use finite element and boundary element methods to solve the above problem for the cases where D is a circular or an elliptical region.

MELNIK, Roderick V N (University of Southern Queensland, Australia)

Mathematical and numerical analysis of hyperbolic models for shape-memory alloys

Using the Leray-Schauder principle we analyse the well-posedness of a general nonlinear model of hyperbolic thermoviscoelasticity describing the dynamics of shape-memory alloys. The model, based on a coupled system of nonlinear partial differential equations, accounts for finite speeds of thermal disturbances by a constitutive relationship implicitly determined from the Cattaneo-Vernotte equation. By a reduction of the model to a system of differential-algebraic equations, we develop an efficient numerical algorithm for the solution of the problem. Computational results on the analysis of thermally and mechanically induced phase transitions in a shape-memory-alloy rod are presented This is a joint work with A J Roberts and K A Thomas.

MELROSE, Gordon (Old Dominion University, Norfolk, USA)

The bending problem for a simply supported strip with internal supports

The problem considered is to determine the stress distribution when a finite width rectangular plate, simply supported along its long edges, and with a pair of collinear internal supports perpendicular to these edges, is subjected to an applied load. Through standard techniques and superposition, the problem is reduced to a mixed boundary value problem, which in turn can be reformulated in terms of a hypersingular integral equation. The integral equation is solved numerically by expanding in terms of Gegenbauer polynomials. Numerical results showing the stress concentration at the ends of the internal supports are given.

MICHELETTI, Stefano (Politecnico di Milano, Dipartimento di Matematica "F. Brioschi", Milan, Italy)

Mixed finite volumes for advanced transport models in semiconductors

In this communication we deal with the two-dimensional numerical simulation of semiconductor devices using advanced transport models. We propose efficient and accurate solvers based on the use of cell-centred Mixed Finite Volume methods derived from the Raviart-Thomas finite elements of lowest degree. This ensures strong conservation of electric field, current and energy fluxes, while nonnegativity of the concentrations and temperatures of the carriers is achieved through a suitable extension of the Scharfetter-Gummel method. Numerical results to validate the newly proposed stabilized method are provided. In particular, a complete electric characterization is carried out for a realistic state-of-the-art n-MOS transistor. This is a joint work with Riccardo Sacco, Politecnico di Milano, Dipartimento di Matematica "F. Brioschi", Milan, Italy.

MICHIELSEN, Bas L (ONERA, France)

A boundary integral equation for high frequency electromagnetic scattering problems

We show uniqueness and existence for a boundary integral equation for electromagnetic scattering problems. The equation is a kind of generalised combined field integral equation based on a parametrix having the same principal symbol as the Dirichlet-to-Neumann operator of the boundary. We benefit from the high frequency localisation of the latter operator to obtain sparse systems upon discretisation. A modified version of the equation is shown to have asymptotically vanishing interactions between "hidden faces," which makes the coefficient matrices even sparser.

MIHÁLYKÓ, Csaba (University of Veszprém, Veszprém, Hungary)

Approximate method for solving a stochastic model of batch grinding

For describing the batch grinding process a partial integro-differential equation is often used which is set up for the density function $v(x,t)$ of the material. One of the auxiliary functions in the equation has a parameter (n), which can be considered as a random variable because of random effects. For solving the stochastic model we elaborated an approximate method based on the numerical solution of equation for fixed n . In our presentation we show the approximate method, we prove its convergence and advantage properties and we illustrate the accuracy of the method by presenting some example. This is a joint work with E O Mihalyko and Zs Ulbert.

MIJANGOS, Eugenio (Basque Country University, Spain)

Multiplier methods for nonlinear networks with side constraints

The minimization of a nonlinear function subject to flow conservation equations, side constraints and simple bounds can be performed by minimizing an augmented Lagrangian function, including only the side constraints. A globally convergent algorithm is designed and implemented using multiplier methods. The performance of this implementation is compared with specialized and general purpose codes.

MIKHAILOV, Sergei E (Wessex Institute of Technology, UK)

Nonlinear functionals interpolation and its application to non-local strength functionals identification

A problem of interpolation of a non-linear bounded continuous functional defined on a closed set S of a Banach space is considered. The functional values are given on a finite number of elements of S and/or on finite-dimensional subsets of S . Several schemes of interpolation of the functional onto S and their convergence are discussed. Results are applied to the identification problem for the strength functionals on the basis of fracture tests data. The functionals are defined on stress fields $\sigma_{ij}(x)$ being functions from L_2 in this application. The functional values are known on a finite number of test stress fields and also on finite dimensional sets associated with the strength surfaces for critical stresses in a body under uniform stress state and for the critical stress intensity factors in a body with a large crack under mixed-mode loading. Interpolation onto all admissible stress fields is discussed.

MITSUMI, Taketomo (Nagoya University, Nagoya, Japan)

GP-stability of two-step implicit Runge-Kutta methods for delay differential equations

GP-stability of two-step implicit Runge-Kutta (TIRK) methods for numerical solutions of systems of delay differential equations (DDES) is investigated. When TIRK is applied to the initial value problem of the linear system of test DDEs given by $y'(t) = Ly(t) + My(t - \tau)$ ($t \geq 0$), $y(t) = b(t)$ ($t \leq 0$), a linear recurrence formula is derived, assuming an interpolation procedure associated for the delayed back values. An investigation of the characteristic equation of the recurrence formula enables us to give a criterion of GP-stability. This is a joint work with Biao Yang, Shanghai Normal University, Shanghai, China.

MIYAKODA, Tsuyako (Osaka University, Japan)

On the computation of the characteristic values of the Mathieu function

The solutions of the Mathieu's equation $u'' + (a - 2q\cos 2x)u = 0$ are expressed in the form of Fourier expansion. Those coefficients satisfy the three-term recurrence relations and are derived according to the values of a and q . The difficulty of estimating the n -th characteristic value a_n is depending on the parameters and the range of x . As for the parameter q and n , we describe how to choose the initial value of the iteration for each characteristic value and study the properties of the iteration formulas.

MIYAZAKI, Teruo (Kokushikan University, Department of Mechanical Engineering, Japan)

Unsteady three-dimensional cascade flow solver using complex temperature gradients

The unsteady three-dimensional compressible Navier-Stokes solver for complicated cascade flowfields with the injection of film cooling air, shock-boundary-layer interaction, and so on, under unsteady and non-uniform inlet flow conditions, is presented. The field governing equations along with initial boundary conditions are reduced to fundamental equations for complex velocities and complex temperature gradients and then solved iteratively. The complex temperature gradients can easily fit thermal conditions in arbitrary locations and make for interchange of necessary informations among the parameters. Numerical examples for a transonic rotor flow and a film-cooling flow were shown successfully.

MOLOKOV, Sergei (Coventry University, UK)

Propagation of stress waves in wires carrying electric current

The propagation of magneto-thermo-elastic stress waves induced by high pulsed currents in metallic wires is investigated both analytically and numerically. The study is related to the exploding wire phenomenon, which plays an important role in pulsed power systems. The stress waves have both mechanical (the electromagnetic pinch effect) and thermal (Joule heating) origin. It is shown that for wires with free ends the magnitude of tensile stress produced by the thermal expansion may well exceed the ultimate strength of material. This leads to the fracture of the wire, which was previously experimentally observed.

MOMBAUR, Katja D (IWR, University of Heidelberg, Germany)

Open-loop stable control of running and hopping robots

Open-loop controlled robots must be able to recover automatically from small perturbations even though these are not actively detected by sensors. We develop numerical optimization methods for the design and the control of such robots and examine biped and monopod robot configurations. Periodic energy or speed optimal motions are determined using a direct boundary value problem approach based on multiple shooting. A stability analysis of the solution is performed based on the Floquet multipliers of the linearized system. We take advantage of the fact that high precision linearizations of the equations are available in the optimization code.

MONTANARO, Adriano (Dipartimento di Metodi e Modelli Matematici per le Scienze Applicate, University of Padua, Italy)

On small-amplitude waves in internally constrained and prestressed linearly elastic materials

For linearly elastic materials, which are internally constrained and prestressed, the conditions of propagation are characterized for small-displacement waves. It is shown that, just as in the unconstrained case, the laws of propagation for discontinuity waves of any given order and for progressive waves are the same. Waves are classified as mixed, kinematic, that are reaction-free or reaction-inactive, and ghost. The conditions of propagation are studied for the constraints of incompressibility, inextensibility, incompressibility together with inextensibility, preservation of orthogonality, and the internal constraints for Kirchhoff plate-like bodies.

MORRO, Angelo (University of Genoa, Italy)

Reflection and transmission through a stratified slab

Time-harmonic waves, generated by an obliquely-incident wave, are considered in a stratified, anisotropic, viscoelastic solid slab. Conditions for nonuniqueness or incompatibility of the direct scattering problem are provided. A detailed analysis is performed of propagation of horizontal waves in isotropic stratified slabs. As is often the case, the solution is found to satisfy a vector integral equation. Here, though, the solution proves to be given by a single scalar function g satisfying a Volterra equation. The explicit form of the reflection and transmission coefficients is established in terms of g . As a check, Fresnel's formulae are recovered in the limit case of slabs of vanishing thickness. This is a joint work with G Caviglia.

MORTAZAVI, Iraj (Mathematiques Appliques de Bordeaux, France)

Pressure field computation using a predictor-corrector method

In this work, the pressure field is computed using a predictor-corrector method for incompressible flows. This method tries to solve the pressure equation under the mass conservation constraint. The method consists of three essential steps. The first step contains a sweeping procedure, that computes an estimated pressure value for all grid points in a progressive way. For this step, pressure gradients derived from Navier-Stokes equations are used. This way, Dirichlet boundary conditions and predicted initial conditions, make easier the resolution of the pressure Poisson equation in the second step. Once convergence is achieved, in the third step, we correct the pressure values at the boundaries by considering interior mesh points and the pressure gradient taken from Navier-Stokes equations. Therefore, this is a predictor-corrector technique, starting with a sweeping calculation and correcting these estimated results, later, by an iterative method which solves the Navier-Stokes elliptic equations. The results of this pressure field computation, that are validated for channel flows, show a fast rate of convergence. This is a joint work with Andr Giovannini, Institut de Mcanique de Fluides de Toulouse, France.

MOURA NETO, Francisco D (Instituto Politcnico, Universidade do Estado do Rio de Janeiro, Brazil)

Heterogeneous porous medium and Darcy's law

We consider slow viscous incompressible flow through a heterogeneous porous medium. We present a general construction for models of heterogeneous porous medium given by families of ϵ -dependent sets with locally varying periodic structures. The parameter ϵ is the ratio between typical pore size and the macroscopic porous medium size. By means of the method of homogenization [E. Sanchez-Palencia, *Non-Homogeneous Media and Vibration Theory*, vol. 127, Lecture Notes in Physics, Springer-Verlag, 1980] and a generalized Bernoulli's theorem, we derive a macroscopic Darcy's law, $v(x) = \frac{K(x)}{\mu}(f - \nabla p)$, and macroscopic incompressibility equation, $\nabla \cdot v$ for the description of the fluid flow. Here v is the velocity of the fluid, μ is its viscosity, p is the pressure, f is the external force and $K = K(x)$ is a spatially varying permeability tensor reflecting the heterogeneous nature of the medium; it is determined by solving microscopic local problems for each point in space taking into account the non constant local structure of the porous medium. This is a joint work with S T R Melo.

MOUTAZAIM, Fathallah (Genie informatique, Compiegne University, Compiegne, France)

Inverse Stefan problem

This study deals with the identification of solid/liquid interface in one phase Stefan problem, in one dimensional case. In many industrial applications, the position of the interface is unknown. Indeed, the phenomena occurring in the fluid are often unknown and cannot easily modelled. We propose in this paper to identify the shape and evolution of the interface using modelling and measurements on the boundary of the solid phase. To solve the problem one uses the least squares regularized method. The resolution of this problem is achieved by the method of the conjugate gradient, which requires the calculation of the gradient. The calculation of the latter, is done by the equation of state sensitivity, compared to interface and its adjoint state. The parameter of regularization is to be chosen according to precision and of stability. This is joint work with Abdellatif El Badia.

MULHOLLAND, Anthony J (Department of Mathematics, Glasgow Caledonian University, Glasgow, UK)

Fractal simulated annealing

The determination of the species composition of a reacting, closed system at equilibrium is a problem in chemical physics which is of major industrial importance. In this talk we will address this problem using a Simulated Annealing algorithm to minimise the Gibbs free energy of the constituent species. One of the advantages of characterising the minimisation space using a fractal analysis is the automatic generation of the cooling schedule and perturbation scheme. We demonstrate the method on a continuous variable problem: the calculation of the Local Thermochemical Equilibrium of combustion gases.

This work is done in collaboration with Professor Jagannathan Gomatam.

MUSCATO, Orazio (Dipartimento di Matematica, Universita' di Catania, Italy)

Check of the consistency of carrier transport models in semiconductor devices with the Onsager reciprocity principle

The increasing miniaturization of modern electronic devices requires an accurate modeling of the energy transport in semiconductors, in order to avoid destructive phenomena in the device. Since a direct numerical integration of the full Boltzmann Transport Equation requires a heavy computational cost, simpler models have been exploited such as Energy transport Model, Hydrodynamic Model, Extended Hydrodynamic Model. In this paper we check the consistency of these models with the Onsager Reciprocity Principle, which is one of the fundamental principles of Linear Irreversible Thermodynamics. Monte Carlo simulations in the homogeneous and inhomogeneous cases are shown. This work is in collaboration with Prof A. M. Anile.

MYASNIKOV, V P (Keldysh Institute for Applied Mathematics, Russia)

Acoustic logging modeling by refined Biots equation

An explicit uniform completely conservative finite-difference scheme for the refined Biots equations is developed for the case of an isotropic heterogeneous porous fluid-saturated elastic medium. This system is modified according to the modern theory of dynamic permeability and tortuosity. The approximate local boundary transparency conditions are constructed. The acoustic logging device is simulated by the choice of appropriate boundary conditions on its external surface. This scheme and these conditions are satisfactory for numerical modeling of an acoustic logging in real axial-symmetrical situation. The developed approach can be adapted also to a non-symmetric case. This is a joint work with Boris D Plyushchenkov, V I Turchaninov (all - Keldysh In-te).

MYERS, Tim G (Applied Mathematics and Computing Group, Cranfield University, UK)

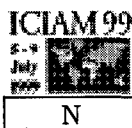
A supercooled Stefan problem relevant to aircraft icing

Ice accretion on surfaces is a significant problem for the aerospace and marine industries as well as electrical power distribution companies, whose overhead lines are frequently damaged (or destroyed!) as a direct result of ice build-up. The aerospace industry in particular is subject to strict control to prevent ice growth on aircraft. Rigorous and time consuming tests must be undertaken during the design and certification of new craft. During flight, when supercooled water is likely to impinge on the aircraft, typically 10% of the generated power may be used to heat susceptible surfaces, to ensure no ice forms. A mathematical investigation of this phenomena, under conditions appropriate for aircraft icing, leads to a supercooled Stefan problem. This problem will be the subject of the talk. The formulation of the one-dimensional problem, at leading order, reduces to a single ordinary differential equation for the ice thickness, which must be solved numerically. The results show that, dependent upon the boundary conditions, the supercooled water may initially all turn to ice and a water layer subsequently appear, ice and water may grow together for all time or water may first appear followed by ice. The first case, where only ice grows initially, shows qualitative agreement with existing experimental results. In two dimensions, the problem becomes more complex, since the water flow plays a significant role in the heat balance. The leading order problem in this case requires the solution of two coupled first order ordinary differential equations, for the ice and water layer thicknesses. Difficulties concerning the flow of this thin layer of water will be discussed and numerical results for the coupled problem presented.

MYŚLIŃSKI, Andrzej M (System Research Institute, Poland)

Shape optimization of contact problems based on fictitious domain method

The paper deals with a shape optimization of the elastic contact problems. The equilibrium state of this contact problem is described by an elliptic variational inequality of the second order. The shape optimization problem for the elastic bodies in contact consists in finding, in a contact region, such shape of the boundary of the domain occupied by the body that the normal contact stress is minimized. The fictitious domain method for solving the state systems described by partial differential equations consists in transforming the original state system defined in the complicated geometry domain into a new system defined in a given fixed simply geometry domain containing the original domain with the same differential operator. This method allows to use fairly structured meshes on a simple geometry domain containing the actual one and fast solvers. In the paper the original shape optimization problem is reformulated in the fictitious domain. Existence of a solution to the shape optimization problem is shown. Necessary optimality condition is formulated. The finite element approximation is employed and the convergence of approximation is shown. The descent gradient method with projection is used as an optimization method. Numerical results are provided.



NAE, Catalin (National Institute for Aerospace Research, Romania)

Solution adaptive approach using unstructured meshes and flowfield parameters

A general approach is presented for accurate and fast CFD computations on 2D unstructured grids using a RANS solver. Starting from an initial grid, constructed using general Delaunay triangulation and initially orientated according to geometric criteria, an initial flow solution is obtained. Using flow parameter like local Mach number or the stream-wise momentum, a metric is build. Using this metric, a new triangulation is build, imposing some external criteria. On this new obtained grid, the old solution is interpolated from the initial grid. Then a new solution is obtained, using initial data from the previous computations. The refinement may continued, using the selected flowfield parameter, until a general performance criteria is fulfilled.

NAKAGAWA, Noritoshi (Hiroshima University, Faculty of Engineering, Japan)

Vibration characteristics of isolator using magneto-spring

The damages of the human body subjected to the vibration of vehicles become important problems with the development of high-speed-vehicle. So far the suspensions of vehicles are designed from the view point of the stroke length, the isolation of high frequency component of vibrations, etc. Therefore, in this study the new vibratin model using magneto-spring is proposed to achieve steady vibration isolation. The magneto-spring model is not easily affected by the frequency, and it can reduce the vibration energy with a small stroke. This is a joint work with E Fujita, H Nakahira, K Chizuka, Y Ogura and O Mahrenholtz.

NAKANO, Yuji (Shiga University, Japan)

On a local causal analysis of time series

Okabe-Nakano (Hokkaido Math. J.,20,1991) constructed Test(S) which states a criterion that time series are a realization of a weakly stationary process. Let $N \in \mathbf{N}$. Let $\mathbf{X}_i = (X_i(n); n \leq N), i = 1, 2, 3$ be three one-dimensional time series. The weak stationarity of these data are tested by Test(S). Here, we propose a method which eliminates the influence of \mathbf{X}_3 from \mathbf{X}_1 and \mathbf{X}_2 . Let \mathbf{X}'_1 be data which left by removing \mathbf{X}_3 from \mathbf{X}_1 . \mathbf{X}'_2 is defined similarly. The local causality between \mathbf{X}'_1 and \mathbf{X}'_2 are defined. A method which judges local causal relations between them is given. We apply this analysis to economic data.

NEDELKOVSKI, Igor (Faculty of Technical Sciences, St Kliment Ohridski University, Bitola, Macedonia)

Computational simulation of steam flow and heat transfer in power plant condensers using finite element method

A method for computational simulation of steam flow and heat transfer in power plant condensers will be presented. The steam flow and heat transfer are modeled by three-dimensional mathematical model for flow of steam-air mixture in the porous media. The model is defined with mass conservation equation for the mixture, momentum conservation equations for the mixture, equation for conservation of air mass fraction, and adequate constitutive equations. For solving this mathematical model a two steps procedure based on the Streamline Upwind Petrov-Galerkin finite element method is developed. By comparison of the results of simulation with experimental results about an experimental condenser, it is confirmed that SUPG finite element method can be successfully applied for solving the three-dimensional mathematical model of steam flow and heat transfer in power plant condensers.

NICOLAS, Jose Antonio (ETSI Aeronauticos, Universidad Politecnica de Madrid, Spain)

Three-dimensional oscillatory boundary layers

Streaming flows generated by oscillatory boundary layers have been widely considered in the literature. In the majority of those analyses the well-known formulas obtained by Schlichting and Longuet-Higgins are used; but these formulas are only valid for 2-D problems. A general three-dimensional analysis of the oscillatory boundary layers, attached to a solid wall and to a free surface has been made. We have derived general formulas for the streaming tangential velocity or stress at the edge of the boundary layer, which generalize the above-mentioned formulas to 3-D motions. Comparison is made with particular results in the literature for specific shapes of the solid walls and unperturbed free surfaces. This is a joint work with Jose M Vega.

NIESSNER, Herbert (Independent, Baden-Rütihof, Switzerland)

Calculation of one-dimensional unsteady flow in pipes with large cross-section variations by the method of Lax-Wendroff with modified flux-correction

The flux-corrected Lax-Wendroff method yields still an efficient algorithm for calculating unsteady pipe-flow. To obtain solutions satisfying conservation laws accurately enough Corberán-Gascón suggest using half-meshes at the boundary requiring minor modifications of flux-correction. Nevertheless oscillations occur with large cross-section variations. In this case Liu et al. propose to transform conserved variables to less fluctuating total quantities prior to flux-correction. We show that this remedy does not work in more extreme cases, but a simple conversion does, and this without deteriorating conservation too much. This is a joint work with Tomas Bulaty of ABB Turbo Systems AG, Baden/AG, Switzerland.

NOWAKOWSKI, Andrzej F (University of Manchester Institute of Science and Technology, UK)

A three dimensional simulation of fluid flow within a hydrocyclone

A method of simulating 3D flow within a hydrocyclone is presented. The proposed technique enables to investigate the effects of inlet geometry on the performance of hydrocyclone. This approach is based on a finite element method combined with a segregated algorithm. An unstructured grid of the tetrahedral elements was generated for a model representation. A solution is obtained using a conjugate gradient type of iterative solver. Some results of flow simulation will also be presented. This is a joint work with R A Williams and T Dyakowski.

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OHTSUKA, Kohji (Hiroshima-Denki Institute of Technology, Hiroshima, Japan)

Theoretical and numerical analysis of fracture in 2D case

The mathematical model of fracture phenomenon is created by Griffith's energy criterion and by using functional analysis. In this model, the force of fracture is the released energy. By finite element method, we want simulate the fracture phenomenon in 2D case.

OINAM, Gourakishwar Singh (Moirang College, Manipur, India)

Frequency modulation of shear waves in liquids under a magnetic field

The nature of elastic wave propagation in media under a magnetic field is discussed by using the conditions of equilibrium. The expressions derived for shear waves depend on the magnetic field and the angle between the directions of wave and the magnetic field showing the anisotropic character. In fluids shear waves are also generated. The changes in frequency due to changes in the magnetic field are discussed in different directions by using the material constants of water. But the change in frequency does not depend on the direction of wave propagation. Analysis of the results shows that magnetic field may be used to modulate frequency of ultrasonic waves.

OKABE, Yasunori (University of Tokyo, Japan)

On a non-linear information and prediction analysis for stochastic processes

As a refinement of the theory of KM_2O -Langevin equations, we construct a local theory for non-linear information analysis for multi-dimensional local stochastic processes. As an application, we develop a non-linear prediction analysis for multi-dimensional local stochastic processes and obtain a non-linear prediction formula for multi-dimensional local strictly stationary processes. This is a refinement of Masani-Wiener's work which has investigated a non-linear prediction problem for one-dimensional global strictly stationary processes.

OLAGUNJU, David O (Dept. of Math. Sciences, University of Delaware, Newark. USA)

Analysis of extensional behavior of viscoelastic filaments

The extensional deformations of viscoelastic filaments have many industrial applications (e.g. fiber spinning, rheometry). In this talk we shall discuss the extensional behavior of viscoelastic fluids described by a number of different constitutive models, including the Oldroyd-B, Johnson-Segalman, Giesekus, Phan-Thien-Tanner, and the Chilcott-Rallison models. These equations will be discussed in the framework of a 1-D thin filament model. We will discuss the effect of rheological parameters such as the Deborah number, retardation parameter, and nonlinear parameters on the stability and necking behavior of viscoelastic threads. For the Oldroyd-B and FENE-CR models, we show that for Deborah number, $De > 0.5$, pure uniaxial extension is linearly stable over a wide range of parameter values due to strain hardening. However, for the other models, the stability is achieved over a much smaller range of parameter values. For $De < 0.5$, all the models exhibit a Newtonian-like behavior, characterized by severe necking at the mid-plane of the filament and ultimately breakup. Finite difference calculations will be presented and compared with available experimental and numerical results.

OLEAGA, Gerardo E (Universidad Complutense de Madrid, Spain)

An explicit solution in plane elasticity

The problem of the unbounded plane with two circular holes in isotropic and homogeneous elasticity is considered. Complex representation and a functional-differential equation are introduced. An algorithm is developed to find the exact elastic field.

This is a joint work with Miguel Ángel Herrero and Juan J L Velázquez.

OLIVAR, Gerard (Universitat Politecnica de Catalunya, Spain)

Modelling switching networks by a one dimensional complex map

In this communication, an approximated mapping for a model of a PWM controlled buck converter working in continuous conduction mode is derived. The new variables are dimensionless, so does the new parameters which are less in number than in the first model. Thus, they can be appropriate to compare the behaviour of the buck converter with other dynamical systems which are described by piecewise-linear vector fields. Finally, a complex map which qualitatively approaches the buck converter behaviour is deduced; it is useful for achieving faster simulations, although some differences from the original system are observed.

ORLOV, Stepan Gennadevich (St Petersburg State Technical University, Russia)

Mechanics of rods as a result of asymptotic analysis of three-dimensional elasticity problem

Static linear elasticity problem for body with small relative thickness splits into one-dimensional problem along arc coordinate and two-dimensional problems in cross section. Settings of these problems for non-homogeneous anisotropic rods are presented. Two-dimensional problems are solved by conventional finite element method. Stress distribution in cross-sections with complex structure is highly non-homogeneous. One-dimensional problem solution method realizes Lagrange theorem for nodal displacements and rotations as generalized coordinates and gives exact solution for loads concentrated in mesh nodes.

Software for analysis of rod systems by asymptotic decomposition method is developed. Magnetic coils are simulated as an example. This is a joint work with Eliseev Vladimir Vasilyevich.

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PANDEY, Bishun D (Ohio State University, USA)

An exact solution to the problem of interaction of a simple wave with a shock wave

A technique is presented to construct an exact solution to a non-linear problem of a gas flow induced by a supersonic piston motion. When a piston moves with a constant supersonic speed into a uniform state of a quiet gas, a uniform shock wave appears spontaneously due to the initial discontinuity of the piston motion. As the shock propagates forward into the quiet gas, the piston is suddenly brought to rest, resulting in the formation of an expansion fan of centered rarefaction waves. When the leading rarefaction wave interacts with the propagating shock wave, the flow field will be divided into three different regions R1, R2 and R3. As a result of interaction the shock becomes non-uniform, and a contact discontinuity appears spontaneously to separate the non-isentropic flow region R3 from the isentropic flow region R2. The flow in region R2 results from the interaction between oncoming and reflected waves; the former propagates along the positive C+characteristics and the latter propagates along negative C characteristics. A class of exact solutions is presented for flows in regions R1, R2 and R3. The trajectories of all boundaries are dictated by the solution itself. Further, the solution enables us to study the decay behavior of the shock waves, and also determines the flow pattern behind a decaying shock wave.

PANFILOV, Mikhail (Oil and Gas Research Institute, Russian Academy of Sciences, Russia)

Nonlinear modes of gas-liquid flow with phase transitions in porous reservoir

Flow of gas-liquid mixture with phase transition in porous reservoir is qualitatively studied. Equilibrium description for mass exchange is used, while hydrodynamics of the process should take into account the nonequilibrium corrections as delaying and hysteresis of relative permeability, which are generated by phase transitions in porous space. The problem of perturbation by a point source is examined using matching asymptotic expansions. The problem is shown to be singularly perturbed with a logarithmic fractional power-value boundary layer. Various modes of flow are detected, with unstable or oscillatory saturation field, as well as the modes of attractor type. The detected laws are used to develop new powerful numerical tools to simulate gas-condensate reservoirs.

PANFILOVA, Irina (Oil and Gas Research Institute, Russian Academy of Sciences, Russia)

Instability threshold of capillary-gravity two-phase flow in porous medium

A non-wetting liquid is invading into the soil saturated by the air under gravity mode, in such a manner, that the capillary forces are contrariwise oriented respectively to the flow direction. This physical model simulates the penetration of various liquid pollutants in the soil. Depending on the Bond number three modes of flow are detected, when the liquid can not penetrate in the soil, can penetrate for any depth, or can penetrate for a limited depth only. These modes are separated by two threshold Bond numbers. Stability analysis accompanied by numerical simulations, has shown the flow to be unstable in vicinity of the higher critical Bond number, where it is developing in form of the rapidly growing fingers. Numerical analysis is based on the percolation-difference method which allows to simulate the physically unstable modes of flow.

PANOVSKI, Sotir (Faculty of Technical Sciences, St Kliment Ohridski University, Bitola, Macedonia)

A method for regulation of work of thermal power plants cooling system

In this paper a system for regulation of the work of power plants cooling system will be presented. With this system permanent work of cooling system with optimal parameters is possible. The work of the system is based on the corresponding method (which will be also explained in the paper) for computer determination of optimal vacuum in condenser in dependence of the power plant working regime. This method is based on the determination of working characteristic of the cooling system in global. The working characteristic of the cooling system in global is formed on the basis of the characteristics of the elements which make the cooling system. On the basis of the working characteristic of the cooling system in global, the optimal vacuum in the condenser is determined i.e. the optimal flow of water in the cooling system in dependence on the power plant working regime and environment.

PARK, Eun-Jae (Dept of Math, Yonsei University, Seoul, Korea)

Mixed finite element domain decomposition methods for parabolic problems

The backward Euler mixed finite element method is considered to approximate the solution of a nonlinear second order parabolic problem. A massively parallel iterative procedure based on domain decomposition technique is presented to solve the resulting nonlinear algebraic equations. Robin type boundary conditions are used to transmit information between subdomains. The convergence of the iteration for each time step is demonstrated. Optimal order error estimates are also derived. Numerical results are given.

PASCA, Daniel (University of Oradea, Romania)

Periodic solutions of second order systems in infinite dimensional Hilbert spaces

We prove the existence theorem of periodical solutions for Hamiltonian inclusions when the Hamiltonian is define in an infinite dimensional Hilbert spaces.

PASQUALI, Aldo (University of Florence, Italy)

Numerical simulations for ring spinning process

In the textile yarn manufacturing process of ring spinning, a loop of yarn rotates about a fixed axis. The surface generated by the rotating yarn is called a "balloon". Here, a numerical method is proposed to integrating a nonstationary mathematical model recently developed by researchers of Florence's University. The method is based on a suitable scaling of the model and uses the finite segments approach, where the equations are discretized by viewing the yarn as a chain of consecutive segments and the forces are concentrated in the connection points. By this method the approximated solution is obtained at each time by solving a unconstrained minimization problem, integrating an ordinary IVP and calculating a definite integral. A careful choice of algorithms for these problems permitted us to obtain a robust and efficient numerical method. Extensive numerical experiments have been performed to study different features of the mechanical process. In particular, we have been able to study the sensitivity of the balloon to several physical parameters and to evaluate a control law of rotational speed of the bobbin in order to reduce tension peaks during the process. This is a joint work with M G Gasparo.

PEGO, Robert L (University of Maryland, College Park, USA)

Spatial wave dynamics of traveling wave surfaces

In several models of three-dimensional water wave propagation we study steady oblique interactions of one-dimensional wave trains. We show that steadily traveling wave surfaces are generated by a wave-like spatial evolutionary dynamics. The talk describes joint work with M Hărăguș-Courcelle, Stuttgart and J R Quintero, College Park & Cali.

PEREIRA, Maria G (GEIASC, Brazil)

Project programming system with multiple resource restrictions

The problem of scheduling activities so as to minimize project duration in the presence of resource constraints is an exceedingly difficult task for projects of even modest size and this problem is commonly encountered by the project scheduler. The purpose of the present paper is to develop a project programming system capable of scheduling activities multiple resource restrictions so that project duration is minimized without violating resource restrictions or altering the sequence of activities. Subsequently, an application of the model is presented in order to verify its uses and to identify its principal difficulties and limitations.

PERGAMENT, Anna Kh (Keldysh In-te for Applied Mathematics, Russia)

Mathematical simulation of the filtration processes in domains with complicated forms

We considered 2D and 3D filtration problem in domains with complicated forms. In order to coordinate a computation model with the reservoir structure of high heterogeneity, it is necessary to use non-regular grids. The method of support operators, allowed us to construct the difference analogs of basic differential operators of the tensor analysis and, subsequently, the finite-difference schemes for equations of the continuum mechanics. These schemes conserve the divergence, positiveness of the elliptical operator, and self-conjugacy. The results of calculations are demonstrated for production fields of Russia. This is a joint work with A V Koldoba, Yu A Poveschenko, and N A Simus, all of Keldysh In-te.

PERNICE, Michael (Center for High Performance Computing, University of Utah, USA)

Hybrid approaches for solution of large-scale systems of nonlinear equations

Nonlinear multigrid and Newton-Krylov methods are both well-suited for solving large-scale systems of nonlinear equations. Since both approaches require selection of components that are problem-dependent, it is unlikely that one strategy will be uniformly superior on a broad class of applications. The strengths and weaknesses of these methods are largely complementary. Linear multigrid methods are excellent preconditioners for Newton-Krylov methods, and have low setup and storage costs compared to other preconditioners such as ILU. Newton-Krylov coarse grid solvers can improve the robustness of nonlinear multigrid schemes. The effectiveness of these hybrid strategies are demonstrated on representative benchmark and practical problems.

PEROTTO, Simona (Politecnico di Milano, Dipartimento di Matematica "F. Brioschi", Milan, Italy)

An adaptive method for Boussinesq equations

The study of the behaviour of short waves turns out to be of great importance in the design of harbours and in the study of estuaries and lagoons. We focus on one of the most common models employed to describe short scale phenomena, i.e. the so-called Boussinesq equations. Boussinesq system arises when the so-called Boussinesq terms are introduced into the shallow water momentum equation. These terms take into account the effects of the wave dispersion. We provide an a posteriori estimate for Boussinesq equations, following the technique introduced by Suli and Houston, and we validate it on some standard one-dimensional test-cases.

PITTERI, Mario (DMMMSA-University of Padova, Italy)

Non-generic concentrations in shape-memory alloys; the case of CuZnAl

It is well known that a solid-to-solid, symmetry-breaking, martensitic phase transition is at the basis of the remarkable properties of many 'active' crystalline materials (for instance, shape-memory alloys). Aided by the detailed kinematical analysis of the phase transitions and of the related twins that can occur in simple lattices, we have recently given some explicit conditions that can improve the twinning ability and hence the macroscopic behavior of a class of shape-memory alloys, i. e. those undergoing a cubic-to-monoclinic transformation. We discuss some explicit theoretical guidelines for determining the special concentrations which may allow for the formation of extra twins in suitable alloys, and thus enhance their memory features. We propose to test such theoretical predictions, by studying experimentally the crystallographic structure, transformation twins, and mechanical behavior of suitable CuZnAl alloys. This approach shows how the theoretical investigation of phase transitions and related phenomena can assist in the search or design of new materials with improved performance. This is joint work with G Zanzotto.

POBEDRIA, Boris E (Moscow State University, Russia)

The problems of computational mechanics of composites

The computational solid mechanics represents a new developing branch of solid mechanics, using computers to get the solution of a task with preassigned accuracy. On every stage, some idealized (canonical) model is analyzed. Due to this, we can, for example, solve the preassigned accuracy the spatial problem for canonical domains. The constitutive relations may be scleronomic or rheonomic. The ways of generalization of the idealized models are described. Sometimes only the discrete form of the constitutive relations exists. The interaction between discretization by time and by space is specifically investigated. The peculiarities of the composite mechanics' problems are distinguished. Non-equalized mechanical properties, physico-chemical interactions of components, optimization control, etc. are discussed.

POLLATSCHEK, Moshe A (Management, Technion, Haifa, Israel)

Graphic interface for model formulations

Algebraic modeling languages (MPL, GAMS, AMPL etc) shorten the time to develop a mathematical optimization model, but it may take weeks or months until a model runs satisfactorily. Further drastic time reduction is possible by graphical notations which proved to be potent in a real-life situation. A prototype will be introduced the input of which is either a flowchart drawn by the user on the screen or a spreadsheet model or the combination of both and the output is the model expressed in an algebraic modeling language of choice.

PONZIANI, Donatella (Dipartimento di Meccanica e Aeronautica, Università di Roma La Sapienza, Rome, Italy)

Perturbative theory and transition to turbulence in wall-bounded flows

Some of the nonlinear features observed in experiments or direct numerical simulations of transition to turbulence in a wall-bounded flow subject to a spatially localized forcing of a given frequency are reproduced in terms of a perturbative theory. The amplitude expansion truncated at second order exhibits two essentially different contributions to the second order correction: one is a superharmonic distortion of a linearized field. The other appears as a steady feature corresponding to streaky structures. The latter is a typical pseudo-resonant response to the quadratic interaction between components of the linearized solution which may be explained in terms of the properties of nonnormal operators.

This is a joint work with D Ponziani, C M Casciola, R Piva, R Piva, Dipartimento di Meccanica e Aeronautica, and F Zirilli, Dipartimento di Matematica, Università di Roma La Sapienza, Roma, Italy.

PORUBOV, Alexey V (Institute of High-Performance Computing and Databases, St Petersburg, Russia)

Exact solutions of nonlinear modulation equations

Some new exact periodic solutions are obtained for coupled nonlinear Schrödinger equations, the complex Ginzburg-Landau equation and the quadratic equations of optical cascading. The profiles of the solutions are quite different from those of the usual envelope wave solutions. In particular, spatial structures for the bounded periodic case vary with time, giving evolution processes close to those observed in nonlinear acoustics experiments. Also the pulse solution of the Ginzburg-Landau equation may exhibit a breather-like behaviour.

POSTAN, Mikhail Ya (Odessa State Maritime University, Ukraine)

Optimal control of multi-nomenclature inventory in continuous production under uncertainty

We analyse a stochastic model of inventory control/production system with multi-nomenclature raw materials and final products which is interpreted as a three-phase storage system. The behaviour of this system is described by a system of linear integral equation (almost surely). The flows of raw materials coming at the first phase (warehouses for raw material storage) are described by the vector Levy process. The case when simple feedbacks are acting in the first phase is considered. For such model some problems of one-stage stochastic programming are formulated (in steady-state regime): a) finding the optimal sizes of raw material's batches; b) optimal distribution of final products between finite number of consumers (points of destination) The problem b) is a type of stochastic transportation problem. This is a joint work with Nikolai N Merculov.

POZDNIAKOV, Vladimir (Institute of Numerical Simulation, Russia)

Resolution of geophysics problems on the base of focusing transformation of seismic multioffset data

At present the common knowledge is that the best way for safe final disposal of radioactive waste is its depositing in stable geological formation. Studies on the suitability of a specific geological objects to be such depository presumes investigations of a wide range of problems the first of which is the presence of destructive zones within the object. We develop an approach that allows to answer this question very reliably. It is based on the fact that any destruction follows by a large cracked area that in its own turns produces strong scattered waves. Our approach allows to recover these areas by means of focusing transformations of seismic data. Detailed numerical and theoretical analysis of its resolving ability is performed. Synthetic and real data are processed.

PREVOST, Xavier (Cranfield University, UK)

3D quasi-steady water flows

This talk deals with the quasi-steady flow of a thin layer of water on a solid surface. The first part deals with the mathematical model and the derivation of the governing equations. The second part deals with the reduction of the equations to a quasi-steady form and their numerical solution. Standard quasi-steady models require a mass balance to close the system. In 2D this is simple to achieve since the water can only flow along a line. In 3D the water position is much more difficult to identify, hence a particular attention is paid to the algorithm required to achieve this. Finally an application of this model to a thin layer of water flowing on an aircraft with ice accretion is described.

This work forms part of the ICECREMO research programme involving four partners, British Aerospace, Rolls Royce, Westland Helicopters and Defence Evaluation and Research Agency. This is a joint work with Dr Chris Thompson and Dr Tim Myers.

PUGH, Mary C (Math Department, University of Pennsylvania, USA)

Long-wave instabilities in thin film equations - blow-up, saturation, and steady-states

Hocherman and Rosenau (Phys. D. 1993) conjectured that longwave unstable Cahn-Hilliard type interface models develop finite-time singularities when the nonlinearity in the destabilizing term grows faster at larger amplitudes than nonlinear effects in the stabilizing term. Specifically, for $h_t = -(h^n h_{xxx})_x - B(h^m h_x)_x$ they conjectured that for $m > n$ finite-time blow-up is possible. Andrea Bertozzi and I show that for such equations, which correspond to a family of equations often used to model thin films in a lubrication context, that in fact the destabilizing term can be stronger (by up to a power of two in the nonlinear diffusion coefficient) yet the solution still remains globally bounded. For the above equation, if $m < n + 2$, smooth solutions are uniformly bounded. We show that this alternate scaling can be easily explained by a conservation of volume constraint and we prove this bound rigorously using energy methods, an entropy dissipation, and interpolation inequalities. Finally we show that when the interface equations permit globally bounded solutions, a weak solution existence theory can be established following similar arguments developed by the authors in recent publications. We also study finite-time blow-up. Richard Laugesen and I study nontrivial steady states of these equations; when do they exist, are they unique, are they linearly stable? We find that one cannot arbitrarily specify the length and area of a steady state, and when there is a steady state with the specified length and area, it may be nonunique. We address similar questions about specifying the area and contact angles, etc.

QUINTELA, Peregrina (Departamento de Matemática Aplicada, Universidade de Santiago de Compostela, Spain)

Mathematical analysis and numerical simulation of a nonlinear thermo-viscoelastic problem arising in aluminium casting

We present a mathematical and numerical study of a free boundary problem arising in casting process. The geometric domain consists of the solidified ingot. The metal is described as a thermo-viscoelastic material. The problem consists of determining the deformations and the stresses, taking into account the metallostatic pressure on the upper boundary due the weight of the liquid aluminium and a unilateral contact condition frictionless with the bottom block. We propose a three-dimensional numerical algorithm and numerical results are given for a real industrial casting. Furthermore, results of existence and uniqueness are given for a simplified problem using monotonicity techniques. This is a joint work with Patricia Barral.

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RADZIUNAS, Mindaugas (Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Berlin, Germany)

Hysteresis phenomenon in numerical simulations of multisectional DFB semiconductor lasers

A mathematical model of a multi-sectional distributed feedback (DFB) semiconductor laser is considered. It is represented by a system of coupled one-dimensional hyperbolic equations describing the propagation of optical waves together with an ODE for the variation of carrier density. The model reproduces the phenomenon of fast oscillating (3-40 GHz) quasi-periodic solutions (Self Pulsations, or SP) which are highly important in optical communications.

A hysteresis of the solution while increasing or decreasing different parameters of the model was observed. Using the same parameters the different types of SP solutions or SP and a stationary solution were detected. The computations are in good agreement with experiments.

RAKOWSKY, Natalja (Alfred-Wegener-Institut for Polar and Marine Research, Bremerhaven, Germany)

Schur complement method as parallel elliptic solver in ocean modelling

Elliptic PDEs with variable coefficients on a domain with complex geometry occur in many ocean models. We present a parallel solver basing on non-overlapping domain decomposition and the Schur complement method. As the PDEs have to be solved repeatedly in a time stepping scheme, setup time can be neglected. Thus, we can effort to calculate the Schur complement matrix explicitly and to derive very efficient preconditioners.

Results for the elliptic PDE in the ice-ocean model BRIOS (Bremerhaven Regional Ice-Ocean Simulation System; Beckmann, Hellmer, Timmermann) indicate that the Schur complement method is well suited for this class of elliptic problems.

RAPPOPORT, Juri M (Russian Academy of Sciences, Russia)

Comparison of numerical methods for $K_{i\nu}(x)$

Several approaches for the numerical evaluation of modified Bessel functions of the second kind with pure imaginary order are introduced and compared on the basis of newly written experimental codes. The methods considered are numerical solution of the differential equation, uniform asymptotic expansions, quadrature, power series, the Lanczos tau-method and the Dziadyck approximation method. Comparisons of accuracy, machine portability and timing are given. Progress is described toward the completion of a new library-grade Fortran-90 code that is based on the comparison results. This is a joint work with D W Lozier and B Fabijonas, National Institute of Standards and Technology, USA.

RASMUSSEN, Henrik Obbekaer (Department of Mathematics, University of Milan, Milano, Italy)

Solution of the energy transfer equation for two-dimensional turbulence

In 1941, Kolmogorov obtained his famous 4/5-law as a solution of the energy transfer equation for three-dimensional turbulence. In this talk, we briefly outline how Kolmogorov's analysis has to be modified in order to handle the case of two-dimensional turbulence. In particular, we show that Kolmogorov's equation is a special case of a more general equation, valid for two- as well as three-dimensional turbulence. For the case of two-dimensional turbulence, this new equation yields inertial-range approximations to the third moment of two-point velocity differences. We thereby confirm the conjecture, made by von Neumann in 1949, that the third moment for two-dimensional turbulence differs fundamentally from Kolmogorov's 4/5-law.

RASUO, Bosko (University of Belgrade, Faculty of Mechanical Engineering, Aeronautical Department, Yugoslavia)

On solving boundary value problem in fluid mechanics by Fourier's method

The influence of transonic wind tunnel walls at 2-D investigations by employing the Fourier's method for solving Dirichlet's problem formulated for a rectangle of test section is given in this paper. In order to preserve the realistic features of flow at the test section's boundaries the boundary conditions, which are to be known to solve this type of boundary value problem, are experimentally determined by measuring static pressure distribution at the vicinity of test section walls. To demonstrate the appropriateness of the presented algorithm for calculation of wind tunnel wall interference at 2-D investigations, the algorithm has been applied to the aerodynamic experimental results from investigations of NACA 0012 airfoil obtained in trisonic wind tunnel in VTI-Zarkovo.

REPETSKI, Oleg (State Technical University, Irkutsk, Russia)

Numerical integration in the 3-D finite element analysis

In any finite element analysis a decision must be made to a number of Gauss points to be specified for the integration of the stiffness and mass matrices. As it is known in the literature, the integration order employed for calculations influence significantly on its accuracy. The use of reduced integration raises frequently the calculation accuracy. However, the principle drawback of reduced integration is so-called "spurious modes" which have no any physical validity. There are different ways to identify spurious modes, but it would obviously be preferable if they did not occur. In an attempt to find a method which would retain the improved performance of reduced integration, but which would eliminate the possibility of spurious modes, a number of techniques for the "selective", "mixed" and "combined" integration were developed. This is a joint work with Prof H Springer, TU Vienna.

REYNOLDS, David W (Dublin City University, Ireland)

Model problem for creep buckling and instability

The dynamic equations for a viscoelastic spring linked to the end of a light rigid rod supporting a heavy weight have the form $\ddot{x} = f(x, y, \lambda, G_0)$, $\dot{y} = \epsilon[y - g(x, G_\infty)]$, where λ is the proportional to the weight applied, ϵ^{-1} to the relaxation time and G_0 and G_∞ are the instantaneous and equilibrium moduli of the standard viscoelastic material constituting the spring. Corresponding to each modulus, there are two elastic problems associated with this system, each having $x = 0$ as an equilibrium. It is a stable solution of the instantaneous problem if $\lambda < G_0$, but a stable solution of the equilibrium problem only if $\lambda < G_\infty$. Our principal interest is the case $G_\infty < \lambda < G_0$, for which $x = 0$ is "metastable". This talk presents results on the asymptotic behaviour of solutions to the viscoelastic equations using a natural free energy. Also, the multiple scale technique of Kuzmak (1959) is used to derive approximate solutions and justify the quasi-static approximation found by Hayman (1978). The stable and unstable manifolds of the equilibrium $(x, y) = (0, 0)$ are also described. This is joint work with Martin O'Gorman.

RICHARDSON, Giles W (Laboratoire Phys. Stat, Ecole Normale Supérieure, France)

Bifurcations in the Little-Parks experiment

We study bifurcations between the normal and superconducting states, and between superconducting states with different winding numbers, in a thin loop of superconducting wire, of uniform thickness, to which a magnetic field is applied. We then consider the response of a loop with small thickness variations. We find that close to the transition between normal and superconducting states lies a region where the leading order problem has repeated eigenvalues. This leads to a rich structure of possible behaviours. A weakly nonlinear stability analysis is conducted to determine which of these behaviours occur in practice.

RIMBEY, Scott E (Educational Testing Service, USA)

Transonic axisymmetric nozzle flows

The boundary value problem governing compressible, steady, inviscid, axisymmetric flow from a nozzle is formulated and solved numerically. The Legendre, or contact, potential formulation is used in the hodograph plane to determine flows where the exit velocity of the gas is supersonic. The entire flow structure is thus transonic. This work extends previous results that were obtained for the analogous subsonic and sonic cases.

ROCHE, Jean R (Université Henri Poincaré Nancy I, France)

Adaptive technique in Newton-like shape optimization methods

Optimization problems that arise in shape optimization are characterised by a cost function depending on geometrical domain and a partial differential equation (PDE) depending also of the geometrical domain. Iterative optimization algorithms are often computationally intensive. We introduce an adaptive strategy to control the approximation accuracy and the approximation cost of a Newton-like numerical procedure. Such superlinear method require a numerical approximation of the second order shape derivatives. We apply this technique to a shape functional which depends on the curvature of the geometrical domain Ω and on a Maxwell equation in the exterior domain Ω^c . To this end we compute a posteriori errors for a boundary elements method.

ROLDAN, Teo (Universidad Publica de Navarra, Spain)

Irk methods for index-2 DAE: Starting algorithms

When semi-explicit differential-algebraic equations are solved with implicit Runge-Kutta methods, the computational effort is dominated by the cost of solving the non-linear systems. That is why it is important to have good starting values to begin the iterations. In this paper we study a type of starting algorithms, without additional computational cost, in the case of index-2 DAE. The order of the starting values is defined, and by using DA2-series and rooted trees we obtain their general order conditions. If the RK satisfies some simplified assumptions, then the maximum order can be obtained.

ROOSE, Dirk (K U Leuven, Belgium)

Numerical stability analysis of steady state solutions of delay equations

The stability of a steady state solution of a delay differential equation is determined by the roots of a characteristic equation. This equation expresses a nonlinear eigenvalue problem, with an infinite number of solutions. In this talk we present a numerical method to compute the rightmost, i.e., stability-determining eigenvalues for a general system of delay equations with an arbitrary number of fixed delays. The method is based on the application of subspace iteration on the time integration operator of the system. The standard algorithm is further modified to improve both the accuracy and the efficiency and to control the errors induced by the numerical time integration and the discretisation of the state space. This is a joint work with Koen Engelborghs, K.U.Leuven, Belgium.

ROOSE, Dirk (Dept. of Computer Science, K U Leuven, Belgium)

Travelling pulse solutions and their stability in anisotropic media

In excitable media, waves are observed to propagate upon a perturbation of a linearly stable, spatially uniform state. We consider anisotropic media described by reaction-diffusion equations with spatially dependent diffusivity. The resulting pulse-like solutions have a varying shape and their computation requires time-dependent calculations. We performed a bifurcation and stability analysis of pulse-like solutions on thin, ring shaped annular domains using two different numerical methods to compute periodic solutions and their stability. We show how these results are related to known results in the limit of vanishing anisotropy and we describe new phenomena. This is joint work with K Engelborghs, K U Leuven and J Krishnan and I G Kevrekidis, Princeton University.

RORRES, Chris (Drexel University, USA)

The turn of the screw: the optimal design of an Archimedes screw

The geometry of an Archimedes screw is governed by certain external parameters (its outer radius, length, and slope) and certain internal parameters (its inner radius, number of blades, and the pitch of the blades). The external parameters are usually determined by how much water is to be lifted and by the site. The internal parameters, however, are free to be chosen to optimize the performance of the screw. In this paper we show how to choose the inner radius and pitch so as to maximize the volume of water lifted in one turn of the screw. Our optimal parameter values are compared with the values used in a screw described by the Roman architect and engineer Vitruvius in the first century B.C., and with values used in the design of modern Archimedes screws.

ROSATO, Vittorio (ENEA, Ente per le Nuove Tecnologie, l'Energia e l'Ambiente, Italy)

Metacomputing for multi-scale modelling of amorphous semiconductors

The direct simulation of the laser melting and recrystallization of an amorphous silicon model system is performed using a large-scale atomistic model described by an empirical potential. The critical regions of the system are periodically "zoomed in" by simulating their behavior using a semi-empirical tight binding hamiltonian. In a metacomputing framework, the master code, which generates the large scale dynamics, distributes the data of the critical regions to different computational platforms which simulate the smaller scale dynamics according to the more detailed interaction scheme. This allows a better description of the system and to obtain information (e.g. on functional properties) not accessible to the model running the large-scale dynamics.

ROSS, Andrew B (University of Strathclyde, Glasgow, UK)

Thin-film flow of a viscoplastic fluid

In this paper we consider flow of a thin film of viscoplastic material on a slowly-varying substrate. Adopting the biviscosity model we investigate flow around a large cylinder and, in particular, derive necessary conditions for the material to yield and give examples of free-surface and yield-surface profiles for several different parameter values. The solution in the singular Bingham limit is also discussed. This is a joint work with B R Duffy and S K Wilson.

ROUSSOS, Nicolette (University of the Witwatersrand, Johannesburg, South Africa)

Applications of lie symmetry methods to nonlinear, dynamic boundary value problems in finite elasticity

The equations of motion arising from dynamic boundary value problems of hyperelastic cylinders and spheres are often highly nonlinear and can subsequently not be solved directly for explicit displacement fields. The curvilinear formulation of finite elasticity is used to derive the equations of motion for the nonlinear radial oscillations of cylinders and spheres with specified strain-energy functions and we apply Lie group methods to find, if they exist, the point and nonlocal symmetries of the equations. A case where the parameter-dependent Lie point symmetries of an equation disappear at higher levels of approximation of the equation is discussed. This is a joint work with D P Mason.

RUBINSTEIN, Isaak (Jacob Blaustein Institute for Desert Research, Ben-Gurion University of the Negev, Israel)

Electroconvective mechanisms in concentration polarization at electro dialysis membranes

Electroconvection is reviewed as a mechanism of mixing in the diffusion layer, responsible for the overlimiting conductance in the course concentration polarization at a cation-exchange electro dialysis membranes. Two types of electroconvection in strong electrolytes may be distinguished: bulk electroconvection, due to the action of the electric field upon the residual space charge of a locally quasineutral electrolyte with nonuniform concentration, and convection induced by electroosmotic slip of either equilibrium (first) or nonequilibrium (second) kind. Theories of electroosmotic slip of both kinds are reviewed and the derivation of a correct slip condition for nonequilibrium electroosmosis, relevant for a developed concentration polarization, is outlined. The following two onset mechanisms for electroconvection of all three above mentioned types are discussed: the onset due to hydrodynamic instability of the quiescent concentration polarization at a homogeneous electro dialysis membranes and the thresholdless onset due to possible short-scale conductive inhomogeneities of the membrane surface. As for the former, both bulk electroconvection and electroosmosis of the second kind yield instability, while this is not the case, for a realistic low molecular electrolyte, for electroosmosis of the first kind. So far, there is no definitive information as to whether the bulk electroconvective instability may develop into a fully-fledged convection, capable of providing a mixing of the diffusion layer at a cation-exchange membrane, sufficient to account for the overlimiting conductance through it. On the other hand, recent calculations show that this is the case for convection induced by electroosmosis of the second kind, through any one of the aforementioned onset mechanisms.

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SADOVSKI, Alexey L (Texas A&M University-Corpus Christi, USA)

A game approach to the solution of nonsmooth problems of mathematical programming

This presentation deals with an application of iterative algorithms for the solution of noncooperative games, developed by author, to solve nonsmooth problems of mathematical programming and optimization. Namely, we are looking for an optimal solution by determining a set of saddle points of Lagrangian corresponding to initial problem of optimization. The whole iterative procedure is based on the solution of polyhedral game. The proposed methods have some advantages such as the simplicity of the each step and the polynomial convergence of the sequence of approximations to the optimal solution. Besides, this approach is derivative free and offers an opportunity to solve problems of mathematical programming and optimization with nonsmooth objective functions and constraints. There is no any need to determine gradients or/and subgradients. This paper presents polyhedral game of the size $(m + 1) \times (n + 1)$, where m is number of constraints and n is number of variables. Speaking of disadvantages of the proposed approach we should mention that convergence is not as fast as a convergence of gradient methods.

SÁNCHEZ-ÁVILA, Carmen (Dpto. Matemática Aplicada. ETSI Telecomunicación. UPM, Madrid, Spain)

Sharp edge signal deconvolution by wavelets

Discrete deconvolution consists of estimating f in $Df + n = \tilde{g}$ where \tilde{g} is an observation vector, n a noise vector, D a matrix corresponding to the action of the observation system, and f the physical magnitude we are looking for. This problem can be viewed as a discrete ill-posed problem. Moreover, we are interested in the case of signal f showing sharp edges. This kind of problem is typical in many fields of applications of digital signal processing, such as seismology, speech coding, etc. In this work we present a wavelet-method for recovering the discontinuities of the original signal. The improvement introduced with this method is illustrated through some simulation examples.

SANTOS, Luis C (Institute of Mathematics and Statistics, University of Sao Paulo, Brazil)

A quick overview of the research on CFD in Brazil

Computational Fluid Dynamics has been proven an important tool for analysis and design in thermo-fluidynamics. As it develops, other areas of knowledge, such as biosciences, and applications, such as the food industry, have been taking advantage of its enormous potential. That's why CFD has encouraged a large number of research groups around the world.

This paper reports the accomplishments of some of the active research groups in Brazil, namely both numerical analysis groups of the University of Sao Paulo, in Sao Paulo and Sao Carlos campuses and the CFD group of the Brazilian Institute of Aeronautics and Space.

SAXTON, Katarzyna (Loyola University, New Orleans, USA)

Nonlinear dissipative-hyperbolic equations modelling propagation of second sound

The model of low temperature heat conduction considered in this talk is an extension of earlier work by R Saxton, W Kosinski and the author, for pure dielectric crystals of sodium fluoride and bismuth. This model accounts for the observable phenomena related to wave-like heat conduction below, and diffusion above a critical temperature. In the paper we will concentrate on the range of temperature where the governing equations are quasi-linear, hyperbolic and dissipative. Three dimensional weak waves are investigated. Under certain conditions the proposed equations are similar to the p-system in the presence of nonlinear damping. This is a joint work with R Saxton.

SAXTON, Ralph (University of New Orleans, USA)

The influence of large data on formation of singularities in incompressible fluids

It is well known that solutions to the two-dimensional Euler equations exist globally in time provided certain restrictions are made on the initial conditions, such as smoothness of data given on a bounded domain. Relaxing these conditions allows the possible loss of regularity after a finite time. We examine a situation in which this does occur.

SCHÄFER, Michael (Department of Mechanical Engineering, Darmstadt University of Technology, Germany)

Numerical simulation of fluid-structure interaction for fluid damped oscillations

The numerical simulation of the fluid-structure interaction is an important field in engineering science. In this paper a weak coupling algorithm is used for the computational fluid dynamics and the structural dynamics problem parts. As an example the oscillation of a torsion spring pendulum in a channel flow is considered for which a damping effect can be observed due to the fluid forces. The moving obstacle causes a change of the fluid domain and consequently of the fluid behavior. Therefore, the movement of the grid has to be taken into account within the Navier-Stokes equations applying a *space conservation law*. This is a joint work with S Meynen.

SCHMIDT, Martin O (Institute for Strength of Materials, Graz University of Technology, Austria)

On the calculation of plastic spin in a model of crystal plasticity based on symmetric tensors

Using the representation theory of compact Lie-groups a yield criterion was developed in (K. Hackl, *Gruppentheorie und Parameteridentifikation in der nichtlinearen, anisotropen Elastoplastizität*, submitted to Z.A.M.M., 1998) which allows to treat the phenomena of crystal plasticity with good accuracy by a single surface model. This procedure is based on symmetric tensors which conflicts with the usually asymmetric expressions of finite anisotropic plasticity, especially concerning the flow rule. A new algorithm, based on a weighted generalized inverse, which determines the symmetric part of the plastic velocity gradient by the group theoretical model and the asymmetric part according to the kinematic relations of crystal plasticity will be presented. This is a joint work with K. Hackl.

SCHWARTZ, Ira B (US Naval Research Laboratory, USA)

Sustaining chaos using basin boundary saddles

We present a general method for preserving chaos in non-chaotic parameter regimes by using the natural dynamics of system. Chaos is preserved by redirecting the flow towards the chaotic region along unstable manifolds of basin boundary saddles, with the use of small infrequent parameter perturbations. General theories will be developed for both smooth and pulsed dynamical systems. Examples of sustaining chaos will be shown in single and multimode laser systems. In addition, redirecting energy away from resonances using sustained chaos in materials will be demonstrated. This is a joint work with Ioana Triandaf, US Naval Research Laboratory, USA.

SCHWETLICK, Hubert (Technical University of Dresden, Dresden, Germany)

A generalized Rayleigh quotient iteration for approximating Eigenpairs of nonnormal matrices

A Rayleigh quotient iteration for approximating eigenpairs of nonnormal matrices is proposed. It is based on a Newton method for bifurcation points of nonlinear equations introduced by Griewank and Reddien which is applied to $F(x, \lambda) = Ax - x\lambda = 0$ and modified such that right and left eigenvector approximations z_k, y_k are updated, too. The method requires to solve two linear systems per step with matrices C_k, C_k^T where C_k comes from $A - \lambda_k I$ by bordering with y_k and z_k^T . The C_k have uniformly bounded inverses so that iterative methods are a choice. It is shown that the λ_k converge locally Q-quadratically, the z_k, y_k R-quadratically. Numerical comparisons with other RQI type methods are given. This is a joint work with R Lösche.

SCOZZAFAVA, Romano (Universita' La Sapienza, Roma, Italy)

Medical diagnosis by coherent probabilistic reasoning

In this paper we apply the theory of coherent inference to the handling of uncertainty in the process of automatic medical diagnosis. No structure and no simplifying and unrealistic assumptions (such as mutual exclusiveness and exhaustivity) is required for the family of hypotheses, supplied by the physician, representing some possible diseases, so that the usual models of Bayesian expert systems cannot help in this context. Our procedure consists in building the family of atoms generated by the given hypotheses: in fact coherence amounts to finding on that family (by solving a linear system) a probability distribution compatible with the given assignment. These steps can be iterated until a final degree of belief, sufficient to make a diagnosis, is reached, and the coherence condition acts as a control tool on every stage. This is a joint work with G Coletti.

SEMENOV, Artem (St Petersburg State Technical University, Russia)

Computer simulation of zigzag-like fatigue crack growth

The direct modeling of fatigue cracks propagation with variation in crack morphology is carried out on the base of continuum damage mechanics concept. The crack initiation and propagation is assumed to occur within the current plane of maximal damage. The various damage measures are introduced and compared for the prediction of the crack growth direction. The special measure is proposed for the description of Forsyth's Stage I crack propagation. The influence of the crack configuration on the effect of crack closure and propagation rate is examined. Elasto-plastic finite element analysis of the steel sharp notched specimens with a single crack under plane cyclic bending is performed for the different cases of loading. Comparison of numerical results and experimental data has been presented and discussed. This is a joint work with S Sähn.

SEO, Jin Keun (Yonsei University, Seoul, Korea)

Inverse conductivity problems: Error estimates and approximate identification

This work studies the global uniqueness and stability questions of the inverse conductivity problem to determine the unknown object D entering $\operatorname{div}((1 + (k - 1)\chi_D)\nabla u) = 0$ in Ω and $\frac{\partial u}{\partial \nu} = g$ on $\partial\Omega$ from the boundary measurement $\Lambda_D(g) = u|_{\partial\Omega}$. We obtain the stability estimates $|D_1 \setminus \bar{D}_2| + |D_2 \setminus \bar{D}_1| \leq C(\|\Lambda_{D_1}(g) - \Lambda_{D_2}(g)\|_{L^\infty(\partial\Omega)}^\alpha + \epsilon)$ for some $\alpha > 0$ when g satisfies some condition if D_1 and D_2 are ϵ -perturbations of two disks. We then drop the condition on g and show that if $\Lambda_{D_1}(g) = \Lambda_{D_2}(g)$ on $\partial\Omega$, then two domains must be very close. This is joint work with E. Fabes and H. Kang.

SERGEEV, Yuri A (Department of Engineering Mathematics, University of Newcastle, UK)

Chapman-Enskog closure approximation in the kinetic theory of turbulent suspensions with application to a gas-particulate pipe flow

The Chapman-Enskog approach is applied to a generalised Fokker-Planck equation for the ensemble-averaged phase-space density of particles to find a closure approximation for the third-order fluctuating velocity correlations in the particle phase of a turbulent dilute gas-particulate suspension. The resulting set of continuum equations is shown to be free of empirical parameters, provided the particles are sufficiently large and the turbulence in both phases is locally isotropic. Special attention is paid to the case where the particle phase is near equilibrium state. The resulting system of continuum equations and boundary conditions is analysed for fully developed flow of dilute but densely loaded suspension in a vertical pipe. The numerical solution of this system shows the bifurcation of flow properties at a certain gas pressure gradient, thus providing an explicit criterion for upward particulate flow. The profiles of particle volume fraction and velocity are calculated, the former demonstrating the phenomenon of particle segregation towards the wall. This is a joint work with David C Swales, University of Newcastle, UK.

SEYRANIAN, Alexander P (Moscow State Lomonosov University, Russia)

On singularities of stability boundaries of linear Hamiltonian systems

Generic singularities of stability domain boundaries of linear autonomous Hamiltonian systems dependent on two and three parameters are studied. A new constructive approach, allowing to determine geometry of singularities with the use of the Hamiltonian matrix, its first derivatives with respect to parameters, as well as eigenvectors and associated vectors at the singularity point, is suggested. Two methods of studying singularities are developed. They are based on the perturbation technique of eigenvalues dependent on parameters and the theory of miniversal deformations of Hamiltonian matrices. Mechanical examples are given. This is a joint work with Alexei A Mailybaev.

SHABOZOV, Mirgand (Tajik National State University, Tajikistan)

N-widths of the some classes of functions analytic in the unit circle

Let X be a Banach space, \mathcal{M} be a convex-central symmetrical set in X , $L_n \subset X$ be a n -dimensional linear subspace, and $\Lambda : X \rightarrow L_n$ be a linear continuous operator. Let $d_n(\mathcal{M}, x)$, $\lambda_n(\mathcal{M}, X)$ denote the Kolmogoroff's and linear n -widths of set \mathcal{M} in X . We consider the space H'_q of functions analytic in $|z| < 1$ with the usual norm. For arbitrary natural r , m and n set

$W_m^r = \left\{ f \in H'_2 : \int_0^{\pi/n} \omega_m^2(z^r f^{(r)}, t)_{H'_2} dt \leq 1 \right\}$, where $\omega_m(\varphi, t)_{H'_2}$ is the modulus of continuity order m of $f \in H'_2$. We prove that $d_n(W_m^r, H'_2) = \lambda_n(W_m^r, H'_2) = \frac{2^{-m}}{n(n-1)\dots(n-r+1)} \sqrt{\frac{m!n}{2(2m-1)!}}$, $r < n$.

SHACHNO, Stepan M (Lviv State University, Lviv, Ukraine)

Difference analogue of Gauss-Newton method and its modifications

For solving the nonlinear least-square problem the difference analogue of Gauss-Newton method is investigated. The regularization of this method is carried out. The modifications of the difference method which under some assumptions are more effective than the initial method are proposed. All of them do not require the evaluation of derivatives. The first modification is based on application of the inverse operator. It enables to receive parallel methods, which can effectively be realized on parallel processors. The another modification uses once calculated operator of derivative on several iterations, that frequently results in reduction of total evaluations. The theoretical research of methods are accompanied by numerical experiments. This is a joint work with Gnatyshyn Oleksandra Pavlivna.

SHADMAN, Dariush (Department of Mathematics, Sharif University of Technology, Tehran, Iran)

On the periodic solution of a nonlinear n th order differential equation

We consider the n th order nonlinear autonomous differential equation $x^{(n)} + f(x, x', \dots, x^{(n-1)}) = 0$, where f is continuous and smooth enough to ensure the existence and uniqueness of solutions of (1) under any set of initial conditions. We shall use a certain transformation to convert the above equation into a system of n second order differential equations $x'' = F_1(x, x')$, if n is even, or into a system of third order equations $x''' = F_2(x, x', x'')$, if n is odd. These systems are then converted into equivalent systems of integral equations. The existence of periodic solutions are then established using the degree argument

SHARMA, B K (Pt Ravishankar Shukla University, Raipur, India)

Existence results for a class of non-linear operators

Many of the questions of Industrial and Applied Mathematics lead to nonlinear problems. These problems require solution. Theory of nonlinear operators provides effective tools to investigate the existence of such solution and calculating its value. A convergence theorem in the form of existence result would be established during the lecture for an special class of nonlinear operators and also their application would be elaborated.

SHEARER, Michael (North Carolina State University, USA)

Undercompressive shocks in thin film flow

Nonlinear hyperbolic conservation laws have solutions with propagating 'shocks' or discontinuities. Classically admissible shocks in scalar hyperbolic conservation laws satisfy a well known 'entropy condition', in which characteristics enter the shock from both sides. Undercompressive shocks, in which characteristics pass through the shock, arise in e.g. combined dispersive/diffusive limits of scalar laws with non-convex flux functions. We show that fourth order diffusion alone produces undercompressive fronts, yielding such unusual behavior as double shock structures from simple jump initial data. Thermal/gravity driven thin film flow is described by such equations and the signature of undercompressive fronts have been observed in recent experiments. Mathematically, the undercompressive front is an accumulation point for a countable family of compressive waves having the same speed. The family appears through a cascade of bifurcations parameterized by the shock speed. This is a joint work with Andrea Bertozzi and Andreas Muench.

SHEVCHUK, Victor (Pidstryhach Institute for Applied Problems of Mechanics and Mathematics, National Academy of Sciences of Ukraine, Lviv, Ukraine)

Approximate calculation of stresses in solids with thin multilayer coatings

This paper suggests the approach essentially simplifying solving of problems of the determination of stress-deformed state of constructions with thin multilayer coatings. It is based on the modelling of such coatings by thin shells with appropriate geometrico-mechanical properties of a coating. In such an approach the influence of thin coatings on the mechanical state of a body-coating system is described by special generalized boundary conditions. This approach gives a possibility of obtaining in certain cases relatively simple analytical solutions of important practical problems for piecewise homogeneous media, which allow to provide a priori qualitative and quantitative estimation of the mechanical state of constructions without complicated calculations.

SHIODE, Narushige (University College London, UK)

Application of graph theory for measuring the inter-connectivity of WWW sites

This study applies a connectivity measure of graph theory to evaluate the network structure of WWW links. It reviews the recent studies on the connectivity of social networks such as Bacon number and Erdos number. We redefine them as discrete, unified case of shortest path finding search in graph theory. We then apply this method to measure the connectivity and accessibility of various Web sites on the Internet, especially those of the academic sites within the United Kingdom as well as those between each country and region in the world.

SHIROTA, Kenji (Department of Mathematical Sciences, Ibaraki University, Japan)

Inverse boundary value problem with the unknown material

The purpose of my talk is to a new numerical algorithm for the inverse boundary value problem for the equation $\nabla \cdot (\gamma \nabla u) = 0$ with the unknown material: Determine the unknown Neumann data and coefficient function by means of the knowledge of simultaneous Dirichlet and Neumann boundary data on a part of the boundary. This algorithm is based on the direct variational method, and a functional is minimized by the method of the steepest descent. In this talk, we confirm the effectiveness of our algorithm by numerical experiments.

SHOJI, Mayumi (Nihon University, Japan)

Calculation of new types of progressive water wave

Water waves on irrotational flow of incompressible inviscid fluid have been the subject of very many researches. However, water waves on rotational flows seem to have been attracted much less attention. We believe that more attention can be paid to rotational waves, since there are many rotational motions in real flows. So we are interested in studying those bifurcation structures. Here we consider two-dimensional steady, periodic surface waves on deep water, under the case where the flow has uniform vorticity. Numerically, we get new bifurcation branches and some new types of limiting wave.

SHURYGIN, A M (Dept of Mech and Math, Moscow State University, Russia)

Statistical analysis and long-term prediction of seismicity for linear zones

I want to report about my method of long-term prediction of seismicity in linear zones. The basis is a model of point field in space and time that can reflect regularities of point locations and reveal latent periodicity. Being extrapolated in future, it gives a prediction function. On retrospective predictions, strong earthquakes locate in maxima of the function. In the future they are considered as signs of danger. Precision of the prediction is less than 10% of the distance from the available bank of data.

SIDOROV, Denis N (Institute of Energy Systems SB RAS, Russia)

About integral model of nonlinear dynamic systems

We use the Volterra functional series $y(t) = \sum_{m=1}^n \int_0^t \cdots \int_0^t K_m(s_1, \dots, s_m) \prod_{i=1}^m x(t - s_i) ds_i$, $t \in [0, T]$

for modelling of nonlinear dynamic systems (see Apartsin A.S., *Some ill-posed problems and their application in energy research*, Sov. Tech. Rev. A. Energy, Harwood Academic Publishers, USA, 1992, Vol. 6, part. 1, p. 65-125 and Apartsyn A.S., Solodusha S.V., *To identification of the asymmetrical Volterra kernels in integrated models of non-linear dynamics*, Proceeding of International Conference on applied and industrial mathematician of memory L A Kantorovich. Novosibirsk, IM SB RAS, 1997, U.1, p. 1 - 13). The cubical model was created. The technique was tested on the problem of construction of an integral model of the heat exchange process, proceeding in a working medium of the steamgenerator.

SIDOROV, Nikolay A (Irkutsk State University, Russia)

Uniformization of the branching solutions and iterations in nonlinear analysis

The N -step iterative method for a computation of branching solutions of the nonlinear equation $F(x, \lambda) \stackrel{def}{=} Bx - R(x, \lambda) = 0$, where B is linear Fredholm operator is given. On every step N linear equations are solved. The value N depends from the structure of the equation of branching. The way of the choosing of the initial approximation and the parameter of uniformization by using the geometry of supported planes and Newton diagrams of branching system is considered.

On the basis of the group analysis (R.S. Mathem. 1988, 11B 883 K, 1991, 12B 1058) modified N -step methods for construction of the parametric set solutions are also given.

SIEGL-MAITZ, Annemarie (Institute for Strength of Materials; Graz University of Technology)

An adaptive finite element procedure for planar elastic problems using wavelets

Wavelets have previously not been used in mechanical problems since the approximation of the boundary destroys the condition of the system of equations to be solved. In (A. Maitz, K. Hackl, *Ein gekoppeltes Finite Elemente-Wavelet-Verfahren für ebene elastische Probleme*, submitted to Z.A.M.M., 1998) a coupled finite element - wavelet procedure has been introduced in order to overcome these difficulties. Based on these results, we proceed by using the wavelet transformation in order to obtain a condition for the adaptive refinement of the strain approximation which also reduces the numerical costs. Another advantage is that we can work now within a standard finite element displacement formulation. The method is demonstrated for an elastic body with a nonlinear nonconvex energy function. In collaboration with K Hackl.

SIMUS, Nathalia A (Lomonosov Moscow State University, Russia)

Mathematical modelling of porous media strain - stressed state occasioned by fluid injection

The strain -stressed state of geology layers occasioned by one - phase filtration is investigated within the quasistationary Biot model. For numerical calculation of the elasticity - filtration coupling problem on non - regular grids computational algorithm based on difference schemes of the support operators method is developed. The process is considered in Romashkinskoye oil set (Tatarstan, Russia) characterized with the existence of listric (curvilinear) faults. The Mohr - Coulomb failure criterion investigated in the faults demonstrated the possibility of occurrence of the seismic event in domain. This is a joint work with V P Mjasnikov, A Kh Pergament, A V Koldoba, Yu A Poveschenko, all from Keldysh Inst. of Applied Mathematics.

SKINNER, Iain M (University of New South Wales, Australia)

Third harmonic generation and modal effects in optical waveguides

Although the generation of a third-harmonic signal by light propagating through a bulk nonlinear optical medium is prevented by material dispersion, modal effects in a waveguiding structure can make it possible. The third-harmonic wave then appears in a higher-order mode. However, analysis of modal properties shows that this possibility only exists for a limited range of wavelengths. This range can be extended by specifying an appropriate non-constant refractive index in the waveguide's transverse direction. The simultaneous presence of self-focussing complicates the analysis, though not the idea.

SLEPYAN, Leonid I (Tel Aviv University and Institute for Industrial Mathematics, Israel)

Dynamic factor in impact, phase transition and fracture

As well known, in a suddenly loaded linear system, the dynamic amplitude is twice as much as the static one while there is no an upper boundary for the dynamic factor (DF) in a nonlinear system. The DF plays an important role in various areas. In particular, the considered questions, 'how to avoid oscillations under an impact' and 'why a phase-transition wave or a crack can (cannot) propagate slowly,' are closely connected with the DF manifestation. The first question is considered in connection with a collision problem. To satisfy the equality $DF = 1$ let the load be monotonically increasing during a time-period and then remain invariable. The minimal period is found which allows a solution to exist as well as the loading rate during this period. The equality, $DF = 1$, can also be true under the viscosity influence. For a standard viscoelastic material a boundary is found which separates the relaxation-creep plane into $DF = 1$ and $DF > 1$ domains. Using a lattice model it is shown that phase transition waves and cracks can propagate slowly in the former domain while only fast waves and cracks can exist in the last one.

SMIRNOV, Georgi (University of Porto, Portugal)

Adsorption integral equation via complex approximation

The relationship between the measured adsorption isotherm and unknown energy distribution function is described by so-called adsorption integral equation, a linear Fredholm integral equation of the first kind. In many cases the equation can be reduced to the Stieltjes integral equation. A new method for solving the Stieltjes equation is developed. The method is based on the ideas of complex approximation and interpolation. The obtained results can be useful for the evaluation of the experimental adsorption energy distribution from experimental data and for organization of chemical experiments.

SMITH, Paul D (Department of Mathematics, University of Dundee, UK)

Electrostatic potential of electrified polygonal plates

The 3-D potential problem for charged polygonal plates may be transformed to a pair of dual integral equations, which in turn may be viewed as a perturbation of similar equations arising from the charged disk. The perturbation depends directly upon the number N of sides of the polygon; as $N \rightarrow \infty$, the perturbation vanishes and the solution tends to that for the circular disk. A practical numerical algorithm with guaranteed computational accuracy can be constructed from this formulation. In addition, approximate analytical solutions can be derived when $N \rightarrow \infty$. In both cases, the capacitance as a function of N is readily calculated. This is a joint work with S S Vinogradov and E D Vinogradova.

SMITH, Ronald (Loughborough University, UK)

Cooperative pollution minimization for two outfalls in an estuary

It is common for there to be more than one wastewater outfall discharging into a narrow (rapidly mixed) estuary. For two outfalls, Bikangaga & Nassehi (Water Research **29**, 1995) showed that matching the two rates of discharge to the flow speeds reduces concentration surges (particularly at slack water) by as much as a factor of 3. Here a constructive algorithm is derived for the two cooperative discharge rates to minimize the peak concentration. Typically, there is a further 30 percent reduction in peak concentration levels.

This work was part of a UK (EPSRC) multi-institution study on pumped outfall discharges.

SØRENSEN, Allan (The Maersk Mc-Kinney Moller Institute for Production Technology, Odense University, Denmark)

A dynamical approach to global optimization

The problem of determining the minimum energy configuration of n equally charged particles constrained to move on the surface of an ellipsoid is a well-known global optimization problem. We will in this paper present a method for computing approximate solutions to this and related optimization problems. The method is based on techniques used in constant temperature molecular dynamics. However, here the temperature is lowered according to some pre-defined cooling schedule and the solution to the optimization problem is obtained in the zero temperature limit when all particles are fixed. The method is compared to a recently developed method based on solving a set of differential algebraic equations which include a simple adhesion force. We find that the method presented here has several computational advantages. This is a joint work with Peder T Ruhoff, The Maersk Mc-Kinney Moller Institute for Production Technology, Odense University, Denmark.

SPENCER, Nicholas K (CSSIP, Adelaide, Australia)

Convex-programming completion of covariance matrices for direction-of-arrival (DOA) estimation

There are significant advantages in using *sparse* linear antenna arrays for DOA estimation, particularly when dealing with more (independent Gaussian) signals than antenna sensors. However, such geometries give rise to partially-specified covariance matrices, which should be completed in some way. For integer-positioned arrays, this involves positive-definite Toeplitz matrix completion; while for noninteger arrays, the problem is Hermitian. Since the optimum maximum-likelihood completion does not yet exist, we propose two other criteria: maximum-entropy and minimum-defective completion. We solve completion using convex programming techniques; while investigating feasibility, optimality, statistical convergence and computational issues. This is joint work with Y Abramovich.

SPIVAK, Alexander (Technological Institute affiliated with Tel-Aviv University, Israel)

Exit problem for Kramer's model

We consider the exit problem for Kramer's model of noise activated escape from a potential well. In this singular perturbation problem the small parameter ϵ is the noise strength (temperature measured in units of barrier height). The stochastic dynamics of the escaping trajectories, conditioned on not returning to a given critical energy contour, are studied analytically and numerically. The distribution of exit points on the boundary of the domain of attraction of the stable equilibrium point in the phase plane is shown to be spread on the separatrix away from the saddle point.

In this problem large deviation theory fails to predict the distribution of the exit point for finite noise. It is shown, both by a numerical solution of the conditioned dynamics and analytically, that most of the probability is located at a distance $O(\sqrt{\epsilon})$ from the saddle point and vanishes at the saddle point.

STAEMPFLE, Martin (University of Glasgow, UK)

Computing the flow of dynamical systems with adaptive triangulation methods

A complete insight into the behavior of a dynamical system can be obtained by investigating the system's flow. This contribution presents a new approach for the numerical computation of the dynamical evolution of multi-dimensional manifolds in time. The new methods are called image methods and are composed of adaptive triangulation algorithms and vertex splines. Image methods operate on a larger class of triangulations and thus show higher flexibility and performance than classical domain methods which are well-known from finite element analysis. The presentation includes theoretical results and numerical algorithms as well as an illustrative example.

STARK, Robert M (University of Delaware, USA)

A conjecture based on the lognormal distribution

Geometric Programs are prized for the engineering design insights that they yield. Cost coefficients, related by the geometric inequality, can be regarded as random variables. The optimality condition suggests that the lognormal distribution may be a natural distribution for the total cost.

STEFANICA, Dan (Courant Institute of Mathematical Sciences, USA)

Domain decomposition methods for mortar finite elements

Domain decomposition methods are general flexible methods for solving the systems of equations arising from the discretizations of PDEs. After the computational domain is partitioned into subregions, a Krylov preconditioner is obtained by solving, in each subregion, problems similar to the original one. We discretize our problem using mortar finite elements, i.e. nonconforming finite elements that allow for a geometrically nonconforming partition of the computational domain and for optimal coupling of different variational approximations in different subregions. We prove convergence estimates similar to those for the conforming finite element case for the FETI method, the balancing algorithm, and the two-level Schwarz algorithm. We present numerical results supporting these estimates.

STEFANOV, Stefan M (Neofit Rilski University, Blagoevgrad, Bulgaria)

Convex separable optimization problems - results, algorithms and some applications

In this work we consider a minimization problem with convex separable objective function subject to a separable convex inequality constraint of the form " \leq " / linear equality constraint / linear inequality constraint of the form " \geq " and bounds on the variables. The three problems are denoted by (C) , $(C^=)$ and (C^{\geq}) , respectively. For each of problems (C) and $(C^=)$, a necessary and sufficient condition is proved for a feasible solution to be an optimal solution to the corresponding problem, and a sufficient condition is proved for a feasible solution to problem (C^{\geq}) to be an optimal solution. Algorithms of polynomial complexity for solving such problems are suggested and convergence of these algorithms is proved. In the Appendix, some computational results as well as some important convex functions for problems (C) , $(C^=)$ and (C^{\geq}) are given. Problems of these types arise in many cases, for example, in scheduling, in allocation of financial resources, in the theory of search, in subgradient optimization, in facility location problems, in the implementation of projection methods when the feasible region is of the same form as the feasible set under consideration, etc.

STEINER, Joseph M (Swinburne University of Technology, Australia)

Trajectory characteristics of planar Grassmann mechanisms

Trajectory characteristics of planar mechanisms consisting of moving links rotating on pivots and intersecting tracks are studied using Grassmann's *Ausdehnungslehre* implemented with *Mathematica*. The combination of this mathematical system representing the underlying algebraic formulation of the mechanism geometry with the symbolic, numeric and animation ability of the computer is a most elegant treatment of this problem. The trajectory shapes are clearly determined by the positions of the tracks and pivots. Trajectories involving cusps, parallelism of link with track, double points at one of the pivots, remoteness, and tininess are considered, and conditions under which these impractical trajectories occur are determined. This is joint work with Gloria Bitterfeld, John Browne and Alan Easton.

STOCKIE, John M (Department of Mathematics and Statistics, Simon Fraser University, Burnaby, Canada)

Modeling gas transport in porous electrodes

Certain types of fuel cells and batteries involve the transport of gaseous reactants through a porous electrode, which is composed of a thin layer of carbon fibre paper. We present a mathematical model for mass transport in gas diffusion electrodes which couples Darcy's Law for flow in a porous medium with equations for mass conservation. Through a combination of dimensional and asymptotic analysis and numerical simulations, we investigate performance issues focusing on the relative importance of convective and diffusive transport and the effect of anisotropy in the fibrous medium.

This is a joint work with Keith Promislow and Huaxiong Huang.

STOJANOVSKI, Vitomir (Faculty of Technical Sciences, St Kliment Ohridski University, Bitola, Macedonia)

Some interpolation methods used during calculations with variable boundary conditions

During the solution of problems involving non-steadystate flow, the question arises as to how to correctly interpolate known boundary conditions which continually change. In general, these boundary conditions are recorded at specific (discrete) intervals, but during solution it is frequently necessary that these conditions be continuously valued for the following reason. The best integration methods use a variable integration step (depending on the intensity of the changes) for the time variable. At each time step, the known boundary values must be as accurate as possible. In this paper three different interpolation methods are used to form a continuous curve from discrete recorded values. These methods are then analyzed with respect to the accuracy of the final solution to the flow problem.

STROM, Staffan E G (Department of Electromagnetic Theory, Royal Institute of Technology, Sweden)

Spectrum of open periodic and waveguide resonators: their significance for the response to external excitations

An approach, which is based on the investigation of singularities in resolvent operators of elliptic boundary value problems, is presented and applied to the solution of applied problems in the theory of resonant wave scattering. The manifestation of nonclassical dispersive properties in linear interaction of eigen modes of the electromagnetic structures are investigated analytically and numerically. Manifestations of nonclassical dispersive properties include inter-mode interactions, the existence of super high Q resonances and regular surface waves in scatterers. Anomalous phenomena, caused by non-traditional features of spectral set elements, such as reflection and transmission for semi transparent structures; total conversion of one wave packet into another resonant conversion of narrow and wide band pulse signals of different types have also been investigated.

This is a joint work with Yura Sirenko and Nataliya P Yashina, Institute of Radiophysics and Electronics, Kharkov, Ukraine.

STRYGINA, Sofia O (Voronezh State Agricultural University, Russia)

Dynamics of relationships between several clinical characteristics of patients affected myocardial infarction

This presentation provides the results of the joint work carried out with V Uskov and S Dement'ev and conducted on looking for factors that play a significant role in the prognosis of myocardial infarction process. Correlation analysis and discriminant analysis are applied to the data set which consist of the the results of the clinical and instrumental investigations of patients with several type of myocardial infarction, which are distinguished with regard to asses of risk. Variables having the most information loadings were selected. Dynamics of relationships between these indicators were analysed.

SUCIU, Elena Alina (Polytechnic University of Bucharest, Romania)

Modeling morphisms for Nagy-Foias diagrams

In the category of Hilbert modules M over a function algebra A we introduce the notion of Nagy-Foias diagram which in case it exists it connects in a special way a minimal subspectral resolution of M with its corresponding minimal subspectral resolution of the adjoint module M_* associated via the minimal spectral dilation of M . We show that there is a one-to-one correspondence between Nagy-Foias diagrams and a class of A -module maps called modeling morphisms. In case A is the disk algebra, the Nagy-Foias diagram expresses the geometry of the space of the minimal unitary dilation of the contraction T which generates the A -module structure on M , while the modeling morphisms are the purely contractive analytic functions. The above correspondence is in this case the Nagy-Foias model based on the characteristic function.

SUGIMOTO, Takeshi (Kanagawa University, Japan)

Stability and self-organization of formation flight

This study presents a core idea of stability and self-organization of formation flight utilized by birds. Air is approximated by incompressible potential flow, and birds are modeled by elliptic wings. Conventional wing theory shows that flow field around wings is described by a newly derived analytic formula by use of complete elliptic integrals. Formation flight is then formulated as a dynamical system of multiple wings interacted each other through induced flow. Physical interpretation of flow field and numerical simulations show the fact: two bird formation is found unstable, while stable V-formation is organized by more than three birds.

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TABATA, Masahisa (Department of Mathematics, Kyushu University, Japan)

Finite element analysis of infinite Prandtl number Boussinesq equations and the Nusselt numbers

Finite element analysis of infinite Prandtl number Boussinesq equations is studied. Especially, we focus on the Nusselt numbers, whose error estimates and computational results are presented. These equations are mathematical models for the Earth's mantle movement and glass flows of industrial production process. Considering the real 3D-computation, we use the P1/P1/P1 stabilized finite element method, which is one of the cheapest element for approximating the velocity, the pressure and the temperature. The boundary condition for the velocity is of slip type, which leads to freedom of rigid body movements in the case when the domain is the Earth. After setting an appropriate function space, we obtain a unique solution and establish an error estimate for the finite element solution.

TAMPIERI, Francesco (CNR Italy)

A generalized Fick law based on fractional derivatives

In general, dispersion in skewed turbulence is described as a non-local phenomenon, which can be interpreted in terms of a flux-gradient relationship (see S. Corrsin, *Adv. Geophys.*, 18A, 25-71 (1974) and J. Lumley, *Phys. Fluids*, 18, 619-621 (1965)) using complex expressions for the eddy diffusivity (see J.C. Wyngaard and J.C. Weil, *Phys. Fluids*, A3, 155-162 (1991)). To properly generalize the Fick's law we propose a model, which expresses the flux in terms of a suitable fractional space derivative of the concentration. This derivative is a non-local, generally non-symmetric, pseudo-differential operator. Inserting this model into the continuity equation, a fractional diffusion equation arises, whose fundamental solution is a Levy stable distribution (see R. Gorenflo and F. Mainardi, *Fractional Calculus and Appl. Analysis*, 1, 167-191 (1998)). This model generalizes the one proposed by Chaves (see A.S. Chaves, *Phys. Lett.*, A 239, 13-16 (1998)). This is a joint work with R. Cesari, F. Mainardi, A. Maurizi, P. Paradisi.

TAN, Roger C E (National University of Singapore, Singapore)

Computation of mixed partial derivatives of eigenvalues and eigenvectors by simultaneous iteration

A new simultaneous iteration method is presented for computing mixed second-order partial derivatives of several eigenvalues and the corresponding eigenvectors of a matrix which depends smoothly on some real-valued design parameters. Numerical results illustrate the viability of the method, and show it to be more stable than a previously published iterative method for derivatives of eigenvectors corresponding to subdominant eigenvalues.

TAN, Yongji (Institute of Mathematics, FuDan University, China)

Parameters optimization of continuous casting problem

This paper introduces how to determine the optimal cooling conditions in second cooling area for continuous casting. In the second cooling area, the temperature distribution should obey some rules. We convert these rules into a cost function. And the Genetic Algorithms are used to minimize this function. Then the optimal spooling scheme has been obtained.

This is a joint work with Haobo Xing.

TANAKA, Atsushi (Computing Service Center, Yamagata University, Japan)

A statistical approach to the travelling salesman problem

In this paper, a new approach to the Travelling Salesman Problem using practical fractal technique is proposed. The Travelling Salesman Problem belongs to one of the most not only fundamental but also useful problem. Since our method is based on a fractal statistical technique, it is quite different from other methods which have been ever proposed. Thanks to taking advantage of the statistical method, a new approach to the Travelling Salesman Problem has been established and it is clarified that our method is applicable to further problems.

TARNOPOLSKAYA, Tanya (CSIRO, Canberra, Australia)

An efficient method for strip flatness analysis in cold rolling

Models of strip flatness in cold rolling consist of coupled models of plastic deformation of the strip, elastic deformation of the roll stack and formation of residual stress, which are usually solved via an iterative procedure. Convergence of standard algorithms is usually achieved by introducing an under-relaxation parameter and a substantial computational cost represents the main obstacle to on-line application of the models. Using a perturbation analysis, we show that the three constitutive parts of the strip flatness model are in fact only weakly coupled and, by taking into account the structure of this coupling, we construct an efficient iterative procedure. This is a joint work with F R de Hoog.

TASSO, Henri (Max-Planck-Institut fuer Plasmaphysik, Germany)

On Lyapunov stability of dissipative mechanical systems

A sufficient condition for linear stability of large dissipative mechanical systems with circulatory forces is derived. According to this condition, dissipative systems which are more than marginally stable without gyroscopic and circulatory forces, remain stable after the addition of weak but finite gyroscopic and circulatory forces. This condition has important applications in plasma physics.

TKACHENKO, Igor M (Polytechnic University, Valencia, Spain)

Orthogonal polynomials and power moment sets for matrix distributions

Transfer functions are boundary values of matrix functions of the Nevanlinna class. The moments of matrix distributions generating such Nevanlinna functions can be obtained using known exact relations and sum rules. The spectral distribution can be constructed using the exact results of the power moment problem for matrix non-negative measures. The matrix versions are to be presented of some classical results of the power moment problem: Systems of orthogonal polynomials; Nevanlinna formulae for all matrix distributions with a given finite set of power moments; Chebyshev -Markov inequalities; Exact bounds for coarse-grained spectral densities and absorption intervals. This is a joint work with Vadim Adamyan, Odessa State University, Odessa, Ukraine.

TOKARZEWSKI, Jerzy (Industrial Institute of Motorization, Poland)

Dynamical interpretation of invariant zeros in degenerate MIMO LTI systems

The zeros are defined as the triples: complex number, nonzero state zero direction, input zero direction. Such definition is closely related with the output zeroing problem. In that spirit the zeros can be easily interpreted even in the degenerate case. Namely, to each complex number we can assign an appropriate real initial condition and an appropriate real input which produce nontrivial solution of the state equation and identically zero system response. A sufficient condition of degeneracy is provided. Other definitions of zeros are discussed. It is shown that those zeros which are defined as the points of the complex plane at which rank of the system matrix drops below its normal rank are also invariant zeros in the sense of the adopted above definition and consequently admit the same dynamical interpretation. Several numerical examples are included.

TOLSTYKH, Andrei I (Computing Center, Russian Academy of Sciences, Russia)

On constructing arbitrary-order difference schemes for parallel processing

The main idea of the paper is introducing linear combinations of N "elementary" difference operators depending on a parameter (or parameters) for obtaining a new operator ("multioperator") which order is proportional to N . Calculations of actions of multioperators on known grid functions can then be carried out in a parallel manner using N processors. As far as spatial differencing is concerned, such possibility is shown to exist if a family of compact upwind differencing operators proposed by the author is used. As a particular cases, $N=3$ and $N=5$ cases providing fifth- and seventh-order discretizations are considered. The stability proof is presented. The resulting schemes are tested against steady-state solutions of the Burgers and the Navier-Stokes equations. The similar idea can be exploited when constructing prescribed-order time integrators. Both theoretical considerations and numerical examples are presented.

TOPIWALA, Diven (Dept of Mathematics, De Montfort University, UK)

The phase retrieval algorithm: A dynamical systems approach

The reconstruction of an object's Fourier phase from its power spectrum, is an important problem in applications from astronomy to crystallography. In principle a discrete object in two or more dimensions with fixed support can almost always be reconstructed from its power spectrum [Hayes,1982]. However, the 'error reduction algorithm', commonly used for this task, often converges to the wrong solution. We analyse this algorithm using dynamical systems theory, studying first small, simple images and then larger images. Bifurcations occur as the target image is varied. We suggest how the performance of the algorithm could be improved. This is joint work with A K Evans, M J Turner and J M Blackledge.

TORRES, María E (National University of Entre Ríos, Engineering Faculty, Argentine)

Integral operators evolution: a new approach by means of q -entropies

Densities arise from the operation over a one-dimensional discrete time system; the study of such systems can be facilitated by the use of densities and the analysis of how successive densities are given by a linear integral operator: the Frobenius-Perron operator. In the present paper we make a first approach to the study of densities evolution in relation with Harvda-Charvat/Daróvczy/Tsallis q -entropies, recently related with fractals, Lyapunov exponents, and nonlinear signals analysis. Their properties in relation with the evolution of Markov and Perron-Frobenius operators are presented. Examples are discussed in the context here adopted.

TRACEY, John (Maths Dept, Heriot-Watt University and Edinburgh Petroleum Services Ltd, Scotland, UK)

Transient two-phase flow in pipes and wellbores

Accurate simulation of the transient behaviour of oil and gas flow is of considerable interest to the oil industry. For instance, transient multiphase behaviour arises in the operation of pipeline systems and in the phase redistribution problem in wellbores. This lecture will describe the results of a collaboration between Edinburgh Petroleum Services Ltd and Heriot-Watt University designed to develop an efficient transient multiphase simulator. A simplified numerical algorithm will be presented for the solution of the governing equations. These consist of conservation laws of mass, momentum and energy.

TSAI, Hsien-Tang (Department of Business Management, National Sun Yat-Sen University, Taiwan)

A reversed two-tailed statistical test

In a standard statistical textbook, a two-tailed statistical test is often introduced to solve hypothesis problems in which the null hypothesis contains an equal sign while the alternative hypothesis contains a non-equal sign. However, we have found some contradictory application examples which are not suitable for this kind of two-tailed test. Therefore, a reversed two-tailed test is proposed for solving those hypothesis problems with an equal sign in the null hypothesis while a non-equal sign in the alternative hypothesis. Some interesting properties of the proposed test will be discussed in detail. Moreover, a lookup table under normality assumption is provided to facilitate the use of the test

TSENG, Shiojenn (TamKang University, Taiwan)

Evaluation of the surface and line integrals of some special functions

A systematic method, which is based on the electrostatics and the Green's function theory, is proposed for the evaluation of the surface and line integrals of some of the Green's function associated with the two- and three-dimensional Laplace and Helmholtz equations. An analytical expression, that can not be derived straightforwardly through usual means becomes retrievable by adopting the present approach. The applicability of the method proposed is justified by four examples often encountered in practice which include a sphere and a planar surface, a sphere in a planar slit, a sphere in a spherical pore, and a sphere in a cylindrical pore.

TUCK, Ernest O (University of Adelaide, Australia)

Inversion of a generalised Hilbert transform

An integral transform \mathcal{H}_y is defined, such that $\mathcal{H}_y f(x) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{f(\xi)(\xi-x)}{(\xi-x)^2+y^2} d\xi$, which reduces to the ordinary Hilbert transform \mathcal{H}_0 when $y=0$, and is useful in some hydrodynamic applications. In these applications, the concern is with inversion of the operator, i.e. determination of $f(x)$, given $\mathcal{H}_y f(x)$. Although \mathcal{H}_y does not seem to be explicitly invertible for $y \neq 0$ (in contrast to $\mathcal{H}_0^{-1} = -\mathcal{H}_0$), it is readily invertible numerically for y less than a certain bound. However, there are issues of a conditioning and precision-loss nature in this inversion process.

TUREK, Zbigniew (ZTUREK Research-Scientific Institute, Warsaw, Poland)

Another alternative approach of getting solutions to some PDEs

In the paper we present a new approach to the solution to some linear PDEs with constant coefficients in a bounded rectangular region. The new approach, contrary to the method of separation of variables (see Churchill R.V. and Brown J.W: *Fourier Series and Boundary Value Problems*, McGRAW-HILL Book Company, New York, 1978), is based only on the Fourier cosine series, independently on boundary conditions. We apply this idea to all components of the PDE according to the way described in (Turek Z: *Application of Fourier Cosine Series to the Solution to Differential Equations*(in Polish), Instytut Naukowo-Badawczy ZTUREK, Warszawa, 1996. and *A New Method of Finding Strong Approximation to Solutions to Some IBVPs*, *Archive of Mechanics*, 49, (3), 573-587, 1997). In this way we transform the PDE into an infinite set of ordinary differential equations (ISODE) for the Fourier cosine series terms to be solved. In the paper we show how effectively the ISODE can be solved for some PDEs describing heat conduction for different boundary conditions. The approach results in Fourier cosine series representations of exact solutions and can be applied to other PDEs. We can successfully solve heterogeneous problems and problems for composites using this idea.

TURNER, Peter R (US Naval Academy, USA)

Image and moving object identification in computer vision

In this paper we present solutions to some of the fundamental problems in computer vision using simple vector-geometric and linear algebraic techniques. The problems discussed are image identification and the three-dimensional location of a moving object in an otherwise known image. The methods used rely on the solution of simple linear homogeneous systems which result from the natural object-image equations. The dimension of these linear systems is small, 6x6 for the classical six-point image identification problem. The model used remains valid for points, lines, or a combination of these. The algorithm is applicable to the most general image projection models. Potential difficulties resulting from coplanarity or colinearity of data points are examined as is the numerical stability of the algorithm.

TWEED, John (Old Dominion University, USA)

Stress intensification due to an edge crack in an anisotropic elastic solid

Integral transform techniques are used to determine the stress intensity factors of a crack at the edge of an anisotropic elastic half space under generalized plane strain conditions. Numerical results are given for the case of a carbon fibre reinforced epoxy in uniaxial tension. This is joint work with Dr. John Tweed, Old Dominion University, USA, Dr. Gordon Melrose, Old Dominion University, USA and Dr. Gilbert Kerr, New Mexico Tech, USA.

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USHIJIMA, Takeo K (Graduate School of Mathematical Sciences, University of Tokyo, Japan)

Convergence of a crystalline algorithm for the generalized curvature flow

Many authors seem to be interested in the curvature-dependent motion. Recently, crystalline algorithm has been investigated actively as an approximation method for curvature-dependent motion. In crystalline algorithm, the curve and the curvature are approximated by piecewise linear curve and crystalline curvature, respectively. We apply crystalline algorithm to the generalized curvature flow; motion by a power of curvature. There exists the solution of generalized curvature flow develops singularity in finite time (blow-up time). In this talk, we show the convergence of the several approximated quantities, especially blow-up time. This is a joint work with Shigetoshi Yazaki.

USHIJIMA, Teruo (University of Electro-Communications, Tokyo, Japan)

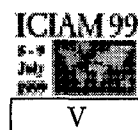
Finite element determination of 2D perfect fluid around a wing

Through finite element computation, we can compute precisely the flow profile of the 2D perfect fluid around the cross section of a wing satisfying Kutta-Joukowski condition at its trailing edge. A proper value γ should be determined numerically in the computation. The value γ , representing the magnitude of the circulation in a normalized sense, is characterized with the aid of the conformal mapping for the wing. The use of natural boundary reduction technique is essential in the determination procedure. Numerical results for NACA23012 and other wings are reported in the presentation. This is a joint work with D Yokomatsu.

VAARMANN, Otu (Institute of Cybernetics at Tallinn TU, Estonia)

Some methods for nonlinear ill-posed equations

Many industrial and scientific problems lead frequently to the solution of ill-posed nonlinear equations. This report deals with the approximate solution of the equation $F(x) = 0$, where F is a Frechet-differentiable operator from a Hilbert space to another. In case F' has the uniformly bounded pseudoinverse it presents a local convergence theorem for a family of methods which includes as special cases the Newton and Levenberg-Marquardt methods as well as ones with successive approximation of the bounded pseudoinverse. If the range of F' is not necessarily closed this report gives a few convergence results on iterative regularization methods based on Gauss-Newton method under certain conditions on a test function and the required solution.



VALUSESCU, Ilie (Institute of Mathematics of the Romanian Academy, Romania)

An operatorial view on infinite-variate prediction

Operator valued L_2 -bounded analytic functions on the unit disc are considered and specific properties, different from the bounded case are obtained. By an appropriate factorization theorem for each semispectral measure there exists a maximal outer L_2 -bounded function. The maximal function permits us to obtain the infinite variate Wiener filter for prediction and the prediction-error operator in terms of its bounded operators coefficients. Similar results can be obtained in the multitime prediction case, but here a special operator valued function arise, which is no longer analytic on the polydisc. Usually white noises here are replaced by colored noises.

VAN DER SCHRIER, Gerard (Netherlands Institute for Sea Research, The Netherlands)

The diffusionless Lorenz-equations; Shil'nikov bifurcations and reduction to an explicit map

A simplified, one-parameter version of the Lorenz (1963) model is obtained in the limit of high Ra - and high Pr -numbers. An extensive range with chaotic motion is found for values of the bifurcation parameter of $O(1)$. For smaller values of the bifurcation parameter a wealth of different periodic solutions is found with a pulse-like behaviour, whereas for larger values of the bifurcation parameter a single smooth periodic solution dominates parameter space. It is shown that it is the Shil'nikov phenomenon that leads to chaos and the complex dependence on the parameter in the model and that homo- and heteroclinic bifurcations dominate the bifurcation structure.

A region in parameter space is singled out where the dynamical system is integrable and the exact solution is given. This solution serves as the limit for strong forcing and appears to be a new integrable case of the Lorenz equations. Approximate solutions are given which are valid for large and small values of the bifurcation parameter. In the latter case an analytical and selfsimilar map is obtained which gives successive periods of the pulselike motion.

VARGA, Laszlo (Hungarian Power Companies Ltd., Hungary)

Approximation algorithms for maintenance scheduling in electric power systems

The preventive maintenance of generating equipment plays an important role in the economical and reliable operation of electric power systems. The schedule of these planned outages is a combinatorial optimization problem. Using the concept of NP completeness it can be proved, that this problem is NP hard so heuristic methods are commonly used in the practical applications. Based on the observation that the maintenance scheduling and the makespan minimization on the parallel machines in the mathematical scheduling theory are equivalent problems, some effective approximation algorithms are presented. Demonstrative examples are shown in which the optimal and sub-optimal solutions will be compared.

VARGAS, C Arturo (IIMAS-UNAM, Mexico)

Thermistor effects on tuned circuit

We consider an electrical circuit with a thermistor. The model is given by a set of three differential equations, two of them are PDE's for the temperature, electrical potential and the voltage. Using multiple-time scales we analyzed the behavior of the thermistor and its the effects on the tuned circuit. This is a joint work with Gregory A Kriegsman.

VARLAMOV, Vladimir V (Departamento de Matematicas, Escuela Colombiana de Ingenieria, Bogota, Colombia)

Long-time asymptotic expansion for the Kuramoto-Sivashinsky equation in a disk

The Kuramoto-Sivashinsky equation arises in the theory of long-waves in thin films, of long waves at an interface between two viscous fluids, in systems of reaction-diffusion type, and in the description of the nonlinear evolution of a linearly unstable flame front. The linear part of the equation describes the interaction of long-wavelength pumping and short-wavelength dissipation, and the nonlinear term characterizes energy redistribution between various modes.

We consider the first initial-boundary value problem for this equation in a circular domain, a natural setting for the Bunsen flame evolution. Applying the eigenfunction expansions method and the theory of perturbations we construct a solution in the form of a series in a small parameter present in the initial conditions. We prove the uniqueness by means of analysing the corresponding nonlinear integral equation. We obtain the uniform in space long-time asymptotic expansion of the constructed solution. Its major term contains the Bessel function of the zero index responsible for the space evolution while the exponential factor emphasizes the time decay.

VÉLEZ-REYES, Miguel (University of Puerto Rico-Mayagüez Campus)

Using subset selection methods for hyperspectral image processing

Hyperspectral imaging sensors provide high-spectral resolution images about natural phenomena in hundreds of closely spaced narrow spectral bands. The expectation is to increase the capability to discern between more classes and increase the classification accuracy. As the number of bands increases, the need for training samples can increase exponentially depending on the classifier being used. Therefore it is of interest to develop methods to reduce data dimensionality with minimal information loss in order to reduce training samples requirements while keeping accuracy. Here we present results on using different subset selection methods as a data reduction stage in a hyperspectral image classification scheme. Subset selection methods are compared in terms of complexity and their effect in classification accuracy.

VENKATESH, Prasana K (Schlumberger-Doll Research, USA)

On a Bayesian method of global optimisation

We present a Bayesian method of global optimisation for obtaining the global optimum of multimodal functions. A Bayesian analysis of Monte-Carlo sample paths on the topography of the functional landscape is performed to derive posteriori estimates of volume fractions of basins of attraction of the set of local optima. A rigorous bound on the posteriori probability of missing the global optimum is derived. Applications on difficult global optimisation problems in nuclear magnetic resonance and in chemical physics are presented. We demonstrate that the computational complexity of our method is superior to simulated annealing and that the method is particularly advantageous for problems with a large number of variables. Comparisons with a deterministic method of global optimisation is also given.

VERMA, Anjulika (School of Mathematics and Computing, University of Brighton, Brighton, UK)

Modelling of an explosion bubble close to a moving structure

The dynamics of an underwater explosion bubble, including its collapse and its interaction with a moving rigid structure, is analysed using incompressible flow theory and a boundary integral formulation. The mathematical formulation of the problem and the numerical methods used to obtain the solution to the axisymmetric problem are described in detail in this paper. Finally we present the results of simulation, using the model, to predict the motion of the bubble close to a moving rigid structure in a number of axisymmetric situations. This is a joint work with P J Harris and R Chakrabarti.

VERNHET, Laurent (Université de Pau et des Pays de l'Adour, Pau, France)

Solution of the Maxwell system with a generalized impedance boundary condition

We consider the boundary-value problem relative to the scattering of a time-harmonic electromagnetic wave for an Engquist-Nédélec boundary condition, which is a generalized Leontovich type boundary condition involving derivatives of the charges. Eliminating the electric field, we design a formulation as a regular elliptic boundary-value problem. This allows to establish existence, uniqueness and regularity properties for the solution to a variational boundary integral equation we suggest to effectively solve the scattering problem.

VILAIN, Claire (INRIA, France and DIM, Chile)

Optimal power flow problem with parallelization of the security's constraints

The Optimal Power Flow Problem is minimising losses of active power over a very high voltage power network by determining the voltage profile and the planning of reactive power compensation devices. This problem is formulated as a nonlinear mathematical program and is solved by using a predictor-corrector interior-point method. Then, we introduce the security's constraints : when the optimal reactive power compensation devices are installed, the voltage during a electrical line's collapse must stay inside the materials limits. We use pvm-scilab for the nonlinear programming of the interior-point method and the parallelization of a collapses set constraints on several processes. This is a joint work with Frederic Bonnans and Eric (INRIA).

VINCENT, Christian (Université de la Réunion, France)

On a comparison of discretization schemes for the Stokes problem

This work is devoted to a comparison of various discretization schemes for the Stokes equations in fluids mechanics. The classical Q1-P0 element with or without stabilization procedures, a new mixed finite element in which the velocity and the pressure are defined on different meshes, the classical marker and cell method and a finite volume scheme are considered. These schemes lead to the solution of saddle point systems which can be transformed into equivalent symmetric positive definite problems for the pressure. We study how the condition number of the (so-called) pressure matrix varies from one scheme to another. This question is of great importance when iterative solutions are considered. Various theoretical and numerical results about the spectrum and the condition number of the pressure matrix are developed. This is a joint work with L Bitar.

VINOGRADOV, Sergey S (Department of Mathematics, University of Dundee, UK)

Wave scattering from elliptic plates

The Method of Regularisation, which was previously used to solve potential problems for elliptic plates, is extended to rigorously treat wave scattering from such shapes. A set of dual integral equations determines the unknown spectral density function. These are regularised by analytical inversion of the singular (static) part. A practical numerical algorithm results from the representation of the unknown function as a Neumann series expansion in Bessel functions. Acoustic and electromagnetic diffraction problems can be efficiently analysed. This is relevant to the design of patch antennas and frequency selective surfaces. This is a joint work with P D Smith.

VINOGRADOVA, Elena D (Department of Mathematics, University of Dundee, UK)

Electromagnetic diffraction from spheroidal cavities

An exact formulation of diffraction from a prolate (or oblate) spheroidal shell with one or two symmetrically placed circular holes, or a longitudinal slot, leads to dual or triple series equations for the scattered field Fourier coefficients. A method of regularisation is extended to solve this new class of equations, involving spheroidal angle functions. Axial electric dipole excitation of such spheroidal cavities is accurately and stably solved, over a wide frequency range, for any geometrical parameters of the scatterer (major-minor axis ratio, angular hole width). The solution is used to compute frequency dependent radiation resistance and far-field-radiation patterns. This is a joint work with P D Smith.

VLASOV, Vladimir I (Computing Center of Russian Academy of Sciences, Moscow, Russia)

A meshless method for solving boundary value problems in 3D domains of complex shape

There is presented a new analytical-numerical method for solving boundary value problems for elliptic equations (e.g. Poisson, Helmholtz, biharmonic, etc.) in 3-dimensional complex-shaped domains. The boundary may contain such geometrical singularities as cones, edges, polyhedral corners, etc. The method ensures very high accuracy not only for the solution itself, but for its derivatives up to singularities also, and for intensity coefficients in the singularities. This accuracy can be checked up with the help of a posteriori estimates obtained in our works. The method possesses exponential rate of convergence. It is based on the use of special systems of functions which reflect adequately the structure of the solution near singularities and possess good approximation properties.

VOLPERT, Vladimir A (Northwestern University, USA)

Mathematical modelling of frontal polymerization

Frontal polymerization (FP) is a process in which a spatially localized reaction zone propagates into a monomer, converting it into a polymer. The process is currently under investigation as a novel method to produce polymers. We develop a mathematical model of FP and determine the structure of the polymerization wave and its propagation velocity as well as their dependence on the parameters of the problem. The mathematical formulation involves the study of traveling wave solutions of parabolic systems. Our analytic results are in good quantitative agreement with both numerical simulations of the model and experimental data.

VORONIN, Albert N (Space Research Institute, Ukraine)

Multi-objective design of combined effect of biologically active substances

A new approach is proposed towards formalized research procedure of combined effect of biologically active substances on biological organisms and systems. The approach is based on original concept of multi-objective theoretical and experimental methods in pharmacology and toxicology. A substances composition offers advantages not found in single substances. When administered to a biological object, its effect must be assessed with the whole set of contradictory criteria. Hence, a method of multi-objective programming is to be employed in the research procedure. We use a new multicriterial theoretical-experimental method underlied by a non-linear trade-offs apparatus. The suggested approach makes it possible to formally assess the effect of the biologically active substances composition in the sense of the contradictory criteria set, and also to accomplish choice between the most agreeable composition values. A new simulation procedure is suggested to minimize the number of animals involved in the experimental research without loss of truth of the trial.

This is a joint work with A V Chubenko, A I Kozlov and T I Nijeradse.

WALHIN, Jean-François (Université Catholique de Louvain, Belgium)

The true claim amount and frequency distributions in presence of a Bonus-Malus system

We use the algorithm of Lemaire and the non-parametric mixed Poisson fit of an automobile portfolio in order to find the true claim amount and frequency distributions that are affected by the presence of a bonus-malus system due to the desire developed by drivers for bonus. This is joint work with Prof J Paris.

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WAN, Honghui (Computational Biology Branch, National Center For Biotechnology Information, Bethesda, USA)

Longest chains in the composite lattices of integer partitions ordered by majorization

A partition of a positive integer l with k parts is a representation $l = p_1 + p_2 + \dots + p_k$, ($p_1 \geq p_2 \geq \dots \geq p_k \geq 0$). Throughout this paper, we use the vector representation for the partition: (p_1, p_2, \dots, p_k) and all partitions are with k parts. Now let $x = (x_1, x_2, \dots, x_k)$ be a partition of m and $y = (y_1, y_2, \dots, y_n)$ be a partition of n . We say y majorizes x , write it as $x \prec y$ or $y \succ x$, if the partial sums of y are at least as big as the corresponding partial sums of x : $x_1 + x_2 + \dots + x_i \leq y_1 + y_2 + \dots + y_i$, ($i = 1, 2, \dots, k$). We denote by $P_{\leq l, k}$ the poset of partitions of all positive integer $\leq l$ with k parts, ordered by majorization. Then $P_{\leq l, k}$ is a lattice. We call $P_{\leq l, k}$ the *composite partition lattice* of l . We develop a fully-efficient algorithm for a finding a maximum-sized chain between two partitions $x \prec y$ in $P_{\leq l, k}$. Based on this algorithm and $P_{\leq l, k}$, we present a new useful complexity measure for biological sequences of length $\leq l$, which overcomes a former limitation that only same-length sequences could be strictly compared for complexity. It is calculated on DNA and protein sequences to illustrate its practical validity as both local and scalable global complexity measures.

WANG, Bei (University of Maryland College Park, USA)

Higher order Godunov scheme for gas dynamics with a nonconvex equation of state

The objective of this work is to develop robust and accurate numerical methods, to validate the numerical schemes, and to extend the 2 by 2 isentropic work of Krispan, Collins and Glaz to 3 by 3 gas dynamics where conservation of energy is included in the system. Additionally, we are interested in the exploration of new phenomenology of two dimensional wave interaction with respect to either shock wave Mach number and wedge angle or constitutive model. We present the numerical results for the simulation of a 3 by 3 gas dynamics with a nonconvex equation of state (EOS); for both two dimensional Riemann problem and oblique shock wave reflection. The computation are performed using second order Godunov-like scheme in which the numerical flux is carefully designed to resolve compound wave structure. The wave interaction and reflection structure are carefully studied. Using numerical comparisons, we have found that our numerical schemes are reasonable in terms of cost, have high resolution capability and appear to be accurate and are capable of generalization to systems involving very complex Riemann problem.

WANG, Hwai-Chiuan (Department of Mathematics, National Tsing Hua University, Hsinchu, Taiwan)

Semilinear elliptic problems in interior and exterior flask domains

In this note we prove that the interior flask domains admits a minimizer if and only if the interior flask domains is thin enough.

WANG, Shin-Hwa (Department of Mathematics, National Tsing Hua University, Taiwan)

An exact multiplicity theorem involving concave-convex nonlinearities and its application to stationary solutions of a singular diffusion problem

We study the bifurcation of positive solutions of the nonlinear two point boundary value problem $u''(x) + f(u(x)) = 0$, $-L < x < L$, $u(-L) = u(L) = 0$, where $L > 0$ is a bifurcation parameter and the nonlinearity $f \in C^2(0, \infty) \cap C[0, \infty)$ satisfies (H1)-(H4). We show that the bifurcation curve has exactly one critical point, a maximum, on the $(\|u\|_\infty, L)$ -plane. Thus, we are able to determine the exact multiplicity of positive solutions. Our results can apply to study number of stationary solutions of a singular diffusion problem, in which we solve a conjecture of Deng [*Nonlinear Analysis, T. M. A.* 18(1992), 731-742].

WATSON, Stephen J (Louisiana State University, USA)

On temporal asymptotics in one-dimensional nonlinear thermoviscoelasticity with phase transitions

The balance laws of mass, momentum and energy are considered for a broad class of one dimensional nonlinear thermoviscoelastic materials. For the initial-boundary value problem corresponding to a specified stress (pressure) on the endpoints held at constant temperature, we present new time-independent a priori bounds on the deformation gradient for initial data of unrestricted size. Subsequent results on the temporal asymptotic behaviour of solutions will also be discussed, with an emphasis on materials which *change phase* (e.g. Van-der-Waals fluid, binary alloys). Simulations of the long time behaviour of solutions based on a discrete paradigm developed by the speaker will also be shown. An additional and novel feature of the theory is that *solid-like* and *gaseous* materials are treated in a unified way.

WERTGEIM, Igor I (Institute of Continuous Media Mechanics, Russia)

Direct numerical simulation of nonlinear structures in non-isothermal channel flows

The three-dimensional numerical study of natural convective flows of incompressible fluid in a infinite plane layer heated from below, in combination with a channel mean flow driven by a horizontal pressure gradient is performed. Two different numerical methods are compared with regard to their accuracy and efficiency : 1) a 3D generalization of the two-fields (stream function and vorticity) approach for plane incompressible flows and 2) a pseudo-spectral approach in the homogeneous directions and 2nd order finite differences method across the layer with primitive variables, used also in its parallel version. The structures of three-dimensional steady and unsteady nonlinear regimes are investigated. The Rayleigh and Reynolds numbers vary from the instability threshold to the high supercritical values. The dependence of the type of structures on flow parameters is investigated. The integral characteristics of flow and heat transfer are determined, as well. This is a joint work with G Alfonsi, B I Myznikova, G Passoni, E L Tarunin and A V Shilkov, partially supported by RFBR grant 99-01-00318.

WEVER, Utz (Siemens AG Corporate Technology, Munich, Germany)

The calculation of sensitivities for optimization problems in fluid dynamics

Advanced applications of CFD for the design process in an industrial environment such as inverse design and optimal design are of increasing importance. Here, it is not sufficient to calculate the usual fluid variables such as pressure, velocity and energy. Also the so-called fluid sensitivities have to be computed in order to get efficient algorithms for design optimization. For the computation of sensitivities we present a numerical scheme which is based on finite volume discretization and on a Roe-solver. Specially the implementation of the wall sensitivity conditions, which are based on the ghost cell technique are discussed. The sensitivity solver is integrated into an industrial turbine blade optimization package. The performance of the sensitivity solver is demonstrated on several examples. This is a joint work with S Stoll and Q Zheng.

WOLOVICH, William A (Brown University, USA)

A complete set of geometric invariants for algebraic curves

Until now, the important problems of determining and constructing a complete set of functionally independent invariants for algebraic curves under various group actions, i.e. Euclidean, affine etc. has remained unresolved, although the invariant counting argument predicts the number of such invariants (see Mundy, Joseph L. and Andrew Zisserman, *Chapter 1 of Geometric Invariance in Computer Vision*, The MIT Press, 1992). Recent results (Unel, M.W.A. Wolovich, *A unique Decomposition of Algebraic Curves*, Technical Note LEMS 166, Brown University, October 1997 and Wolovich, William A. and Mustafa Unel, *The Determination of Implicit Polynomial Canonical Curves*, IEEE PAMI, Vol.20, No.10, October 1998) that we have obtained in algebraic curve theory have now enabled us to solve these problems in a very intuitive way employing some powerful and rich geometric techniques. Unique implicit curve decompositions are developed first and then "non-visual" feature points and lines are derived from the decomposed algebraic equations. Based on the geometry of these features, a complete and simple geometric set of functionally independent invariants under Euclidean and affine transformations are identified and constructed. The results presented can be used in many practical situations, including model-based vision, object identification and pattern recognition applications. This is joint work with Mustafa Unel.

WYATT, Katherine (Logic Based Systems Lab, Brooklyn College, City University of New York, USA)
Maximizing hedge effectiveness under *FASB 133* accounting standards

New U.S. accounting standards for financial derivatives (*FASB 133*) mandate on-balance sheet reporting and the designation of hedged item - hedging derivative pairs for reporting offsetting gain or loss on financial statements. A program that uses disjunctive constraints to model the criteria for hedge accounting across all types of financial instruments and against allowable risks is presented. The program has a piecewise linear objective function, and uses standard risk management reports as input. A linear relaxation of the disjunctive constraints models compliance for most hedges against market risk. Computational results for a trading portfolio are reported.

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XANTHIS, Leonidas S (Centre for Techno-Mathematics & Scientific Computing Laboratory, University of Westminster, London, UK)

Robust iterative methods for thin elastic shells, plates and rods

We address the fundamental question of how to solve efficiently 3D large-scale elasticity problems for thin structures of arbitrary geometry, e.g. shells, plates and rods. We show that by invoking the *Ovtchinnikov-Xanthis's (OX's) Inequality* - the *only* Korn's type inequality providing pivotal information for the radical improvement of the performance of iterative methods for thin structures - we can establish an effective and unified framework for developing robust iterative methods for thin structures with convergence rate independent of both the thickness and the discretisation parameters [see e.g. Proc. R. Soc. Lond. A 453 (1987) 2003-2016 and 454 (1998) 2023-2039]. This work is joint with E E Ovtchinnikov.

XENOPHONTOS, Christos (Department of Mathematics and Computer Science, Clarkson University, Potsdam, USA)

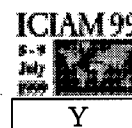
Application of the p -version of the finite element method to elasto-plasticity with localization of deformation

We discuss the use of the p -version of the finite element method applied to elasto-plastic problems, for capturing sharp (but continuous) deformation gradients. Such localized deformation occurs in, e.g. granular materials such as sand. The deformation theory of deviatoric, linearly hardening elasto-plasticity with an iterative, displacement based finite element framework is used. The focus of this work is on assessing the applicability of the p -version of the finite element method to the analysis of localized deformation with continuous strain and displacement fields. Presented examples will show that with proper mesh design, this method can be very a effective and computationally efficient tool for this type of problems. Possible extensions of the work will also be discussed.

YAKOUBENKO, Tatiana A (Moscow State University, Moscow, Russia)

Averaging of processes in periodic media with periods of different orders in the different directions

Homogenization theory is applied to obtain the effective equations for large scale processes in periodic media. Magnitudes of periods in different directions are of different orders. The smoothness of the coefficients of the original equations is not supposed. The asymptotic explicit formulae for averaged media moduli are derived and strictly justified. In particular, anisotropic media with long thin pores of arbitrary form are considered. Comparison of the values of effective moduli obtained by the derived formulae and by numerical solution of the original problem is given.



YAKUSHEV, Vladimir L (Institute for Computer Aided Design, Russian Academy of Sciences, Moscow, Russia)

Investigation of prebuckling and postbuckling stable forms of shells in view of initial imperfections

An effective computing algorithm for a solution of the non-linear problems of shell deformation and stability permitting to discover the upper and lower critical loads, steady prebuckling and postbuckling states in view of initial imperfections and non-linear properties of a material is presented. A basis of the algorithm is the method of an additional viscosity permitting to construct convergent iterative processes, including critical loads. In this case, there is no necessity to change solution parameters and to chose specified procedures for bypassing of singular points. Special conditions were found at which the continuity of a solution on time was ensured at passage from the prebuckling to the postbuckling stable state. An adequacy of stability criterions for the viscous and dynamic equations was proved. For square in a plan cylindrical panel a series of calculations was carried out in view of initial geometric imperfections. The things turned out for the considered shell there was a restricted number of the stable postbuckling forms.

YAMANE, Toshiyuki (University of Tokyo, Japan)

On a non-linear deterministic analysis for complex time series

As an application of the local theory for non-linear information analysis, we develop a non-linear deterministic analysis for local stochastic processes and pursue a non-linear deterministic analysis for some concrete complex time series in natural phenomena, life phenomena, technological phenomena and social phenomena. This is a joint work with Yasunori Okabe.

YASHINA, Nataliya P (Institute of Radio Physics and Electronics, Kharkov, Ukraine)

Novel computer-aided methods in the time-domain theory of periodic and waveguide-type open resonators

New rigorous and efficient methods oriented to the numerical analysis of transient processes in open periodic gratings and waveguide resonators are presented. The approach is based on the description of scattering characteristics in terms of boundary and transport operators of non-stationary fields described in terms of an "evolutionary basis". This basis characterizes fields in e.g. regular waveguide sections uniquely. The versatility of the algorithm is enhanced by the fact that they do not change qualitatively within rather wide band of geometrical parameters of key building blocks. The results enable us enlarge considerably the range of problems that can be solved in rigorous way and provides the possibility to analyze discontinuities with arbitrarily shaped boundaries and containing locally inhomogeneous regions. This is a joint work with Yura Sirenko, Institute of Radio Physics and Electronics, Kharkov, Ukraine.

YASSINE, Boubendir (Cerfacs, UMR MIP INSA-CNRS-UPS, Toulouse, France)

Boundary integral-domain decomposition method for solving the Helmholtz equation

In this paper, we present a non overlapping domain decomposition method applied to a scattering waves problem. We consider Helmholtz equation in an unbounded domain with an impedance condition. Sommerfeld radiation condition is also imposed. Integral equations appear as a very appropriate method for solving this kind of problems. We use an algorithm of domain decomposition based on an iterative method, where unknowns are defined on the interfaces. Particulary, we show how to recover the trace. Some numerical results validating the approach will be presented.

YAZAKI, Shigetoshi (Graduate School of Mathematical Sciences, University of Tokyo, Japan)

On the crystalline algorithm for the curvature-dependent motion

In many research fields, moving boundary problem is an important theme. The typical example is the motion by mean curvature which has been extensively investigated. Our objective is to construct a numerical scheme for computing moving boundaries. By using crystalline algorithm, we have computed the motion of convex curves whose normal velocity is proportional to a power of curvature, and proved its convergence. In this talk, we present crystalline algorithm can be extended for computing the motion of non-convex curves. We also show the reliability of the scheme. This is a joint work with TaKeo Ushijima.

YÚNUSI, Mahmadyusuf K (Tajik State National University, Dushanbe, Tajikistan)

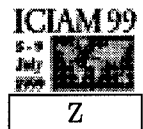
Workers potential function and its applications

The Worker potential function is simulated and investigated. It is shown that this function is a solution of a special class of partial differential equations. When the workers potential function is only of a function of age, we are obtain explicit solutions. Such an approach explains many unknown characteristics of economics(for example, age factors in productions processes). The Workers potential function is also used for more general models in Economics.

ZAFER, Ağacık (Middle East Technical University, Ankara, Turkey)

The controllability of boundary-value problems for quasilinear impulsive systems

The problem of the control of boundary-value problems for quasilinear impulsive systems is investigated. We are considering not only fixed but also variable moments of impulse control. A comparison method is used to investigate the systems with variable moments of impulse actions.



ZALTZMAN, Boris (Jacob Blaustein Institute for Desert Research, Ben-Gurion University of the Negev, Israel)

Electroosmotic slip of the second kind and instability in concentration polarization at electro dialysis membranes

Slip condition for the nonequilibrium electroosmosis (electroosmosis of the second kind), relevant for a developed concentration polarization at an electro dialysis membrane, is derived through a boundary layer analysis of the appropriate convective electrodiffusion problem. Linear hydrodynamic stability of the quiescent concentration polarization in a diffusion layer at a cation exchange electro dialysis membrane under the passage of a normal electric current is studied. It is shown that electroosmotic slip of the second kind yields instability for realistic conditions. Numerical calculations for the resulting nonlinear convection show that the latter provides an efficient mixing mechanism for the diffusion layer, capable of accounting for the overlimiting conductance in concentration polarization at a cation exchange membrane.

ZERNOV, Oleksandr E (Odessa State Polytechnic University, Ukraine)

On continuously differentiable solutions of the singular initial value problem

The following singular initial value problem is under consideration $a(t)x'(t) = F(t, x(t), x'(t))$, $x(0) = 0$, where $a(t) = \text{diag}(a_1(t), \dots, a_n(t))$, $a_i(t) \rightarrow 0$, $t \rightarrow 0$, $i = \{1, \dots, n\}$. Existence of continuously differentiable solutions with needed asymptotic properties when $t \rightarrow 0$ is being proved. If certain conditions are fulfilled, than the number of such solutions is being determined too. The investigation methods are elements of functional analysis and qualitative theory of differential equations joint together.

ZHANG, Wen (Department of Mathematics and Statistics, Oakland University, USA)

Numerical simulation of microstructural evolution in sintering

Sintering is a widely used process in materials manufacture. At the microstructural level, essentially the sintering process can be modeled by a combination of surface diffusion and grain boundary diffusion. The movement of the surface is driven by curvature, modeled by a surface Laplacian. This mathematical model for the mass results in a fourth order nonlinear time dependent parabolic partial differential equation with moving boundaries (the particle surfaces) which are to be determined. We extend the model to complex particle geometries, and we show how to design a computational model using the method of lines for integration in time. Numerical results from sequential and parallel computations will be presented and discussed.

ZHELUDEV, Valery A (School of Mathematical Sciences, Tel Aviv University, Israel)

On classification and recognition of acoustic signals by wavelet methods

The goal of the work was the development of tools for the classification and recognition of acoustic signals emitted by moving vehicles. The key issue was the extraction of characteristic features of the classes involved. For that purpose we used the wavelet packet analysis. As the signature of a class we employed a combination of energies of a few most discriminating blocks of the wavelet packet decompositions of signals. The adaptive algorithm for the selection of such blocks was developed. As a decision making module we used conventional classifiers such as LDA and CART. Series of in-the-field experiments confirmed high efficiency of the tools developed. This is a joint work with Amir Averbuch.

ZHENG, Qinghua (Siemens AG Munich, Germany)

Multiframe technique for flow problems with time varying geometries

For instationary flow problems with complex or time varying geometries in 3D, a multiframe technique based on Cartesian grids has been developed. Geometrical objects with different velocities are handled within different frames and possibly different fine grids. The discretization at wall boundaries ensures mass conservation. Data in overlapping regions are consistently updated. For each frame, a standard flow solver can be used. We have applied this technique to several test cases, e.g. to the case of a train passing an object and to the simulation of the compressible flow interaction between rotating and stationary turbine rows.

ZHILIN, Pavel A (The St Petersburg State Tech. University, Russia)

Multi-spin continuum mechanics and modified electrodynamics

The multi-spin continuum is an extension of the Cosserat continuum (single-spin continuum). The report presents a general theory and its applications to the derivation of the equations by Klein-Gordon, Schrodinger, and Maxwell. This means that the mechanical interpretation is given for each of these cases. Note that the modified electrodynamics follows directly from mechanics and contains two velocities of signal propagation. Classical electrodynamics follows from modified theory if the more high velocity strives to infinity. It is shown that modified theory allows avoiding some paradoxes of classical theory.

ZHMAKIN, Alexander I (A.F.Ioffe Physical Technical Institute, St Petersburg, Russia)

Adaptive multigrid methods for steady viscous flows on unstructured grids

A number of multigrid methods is applied to solution of steady low-Mach number Navier-Stokes equations. Finite volume method on adaptive unstructured or hybrid grids with co-located variables arrangement is used. Among others, algebraic multigrid methods and global solution adaptation coupled to the regular grid refinement are considered. Implementation following object oriented approach resulting in an efficient unified processing of hybrid structured/unstructured and conforming/nonconforming grids is discussed. Examples of 2D and 3D computations of flow and deposition in real-life epitaxial reactors used for growth of semiconductor materials are presented. This is a joint work with S K Kochuguev and D Kh Offengeim.

ZHU, Jianping (Mississippi State University, USA)

On an efficient higher order algorithm for solving partial differential equations

An efficient high order method for solving time dependent partial differential equations will be discussed in this talk. It is based on standard five-point difference stencil that has been typically used in second order methods for solving convection-diffusion equations in two-dimensional domains (seven-point stencil in three-dimensional domains). The new method is fourth order accurate in space and only requires solutions of systems of tridiagonal equations. Furthermore, it does not use the first and second order derivatives as unknown dependent variables as in the traditional compact finite difference algorithms, thereby substantially reducing the computational complexity. Numerical results will also be discussed in the presentation to demonstrate significant accuracy and efficiency improvement.

ZIEN, Tse-Fou (Naval Surface Warfare Center, Dahlgren, Virginia, USA)

An integral method for skin friction and aerodynamic heating calculation

An integral method is presented for approximate calculations of skin friction and heat flux on aerodynamic bodies. It is a refinement of the Karman-Pohlhausen (KP) momentum integral method. The basic idea is to use an integral expression for such a quantity, derived from the integrated form of the pertinent conservation equation. The quantity of interest is thus given by integrals of the approximate solution assumed in the calculation instead of taking its derivative as in the classical KP method. Improvement in accuracy is remarkable. Examples of application include the Falkner-Skan equations, flow in the melt-layer in an ablation model, and some phase-change conduction problems, and results are compared with exact and the corresponding KP solutions to determine the merits of the method.

ZIMMERMANN, Wayne J (Texas Woman's University, Denton, USA)

A computational model to estimate the probability of impact with space debris

The focus of this paper is to provide two models that estimate the probability of an impact between an operational device and a harmful space debris particle.

The paper begins with a review of the various sub-problems. The review includes the following models: following models: the hyper-velocity impact model, the explosion model and its associated mass/velocity distribution model, the debris cloud evolution model and the debris density model. The problem of integration of the various sub-modules is discussed. The resulting model is then used to determine the flux, an impact count. Once the flux has been determined it can be used to estimate the probability of an impact between and an orbiting satellite and a significant debris particle.

ZIOLKO, Mariusz (Department of Electronics AGH, Poland)

A Wavelet-Galerkin approximation of hyperbolic partial differential equations

The Galerkin method is used to approximate the solution of the initial-boundary value problem for a set of first order hyperbolic partial differential equations (PDE). The wavelet series is derived on the interval from compactly supported Daubechies wavelets. The semidiscrete Galerkin method leads to a set of ordinary differential equations (ODE). The boundary condition are incorporated into the ODE. The initial conditions for the ODE are calculated from the initial conditions for the PDE.

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